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THE PARTIAL OXIDATION OF n-BUTANE IN A  
PLUG FLOW REACTOR

BY

NORMAN E. ANDERSON

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES  
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UNIVERSITY OF ALBERTA  
FACULTY OF GRADUATE STUDIES

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance a thesis entitled THE PARTIAL OXIDATION OF n-BUTANE IN A PLUG FLOW REACTOR submitted by Norman E. Anderson in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Chemical Engineering.



## ABSTRACT

The study of the partial oxidation of n-butane in a plug flow reactor is a continuation of the overall investigation on the utilization of hydrocarbons. A reactor was designed and constructed to study the effect of residence time on the overall reaction at various temperatures, pressures, and oxygen concentrations.

Experiments were carried out at three temperature levels of 685, 705, and 725°F and indicated the dependence of the induction period on the inlet temperature. Runs were also made at four different inlet oxygen concentrations to study its effect on the overall reaction.

The reactions gave a 60 per cent conversion of the n-butane reacted to olefins for most of the runs. Only 10 per cent of the n-butane that reacted went to carbon oxides. Of the remaining 30 per cent, 10 per cent went to lower molecular weight hydrocarbons and 20 per cent to oxygenated products. The oxygenated products consisted of aldehydes, ketones, and alcohols.

The gas temperature in the reactor for any run remained fairly constant during the induction period and then increased rapidly to a peak temperature approximately 400°F above the inlet temperature. After the period of rapid reaction the gas phase temperature decreased gradually because of heat transfer from the gas to the reactor wall.







## ACKNOWLEDGEMENTS

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## INTRODUCTION

The partial oxidation of hydrocarbons is complex due to the number of reactions taking place simultaneously, but is of industrial and academic importance. Industrially, the reaction is an important source of oxygenated products such as aldehydes, ketones, alcohols, and acids. In the past few years, the partial oxidation has become an important process for producing unsaturates from saturated hydrocarbons.

The main research interest in the partial oxidation is due to its industrial importance. A knowledge of the effect of temperature, pressure, reactant concentrations, and an understanding of the reaction mechanism are valuable assets for process design and control. Even though much work has been done on the partial oxidation of hydrocarbons in the vapor phase, much remains to be done before the effect of all reaction variables is understood and the mechanism known.

As part of the continuing study on the utilization of hydrocarbons the University of Alberta has been carrying out an investigation on the partial oxidation of n-butane. In 1950 Duthie(11) designed the initial reactor and carried out preliminary experiments. Dalla Lana(9), in 1953, continued the work with the spiral reactor and investigated the effect of pressure, residence time, and reactant concentrations on the overall reaction. In 1960 Musgrove(27) used a variable length reactor to study the effect of temperature and residence time





at constant mass velocity on the partial oxidation reaction.

A survey of the literature published on the partial oxidation of hydrocarbons indicated that more information was required on the effect of residence time on the reaction. The majority of the work has been done with sampling at the reactor exit only and varying the residence time either by changing the flow rate through the reactor or by changing the reactor length. As a result, it was decided to design and construct a reactor that allowed multiple sampling along its length, provided accurate gas and wall temperature profiles, and allowed accurate control of temperature, pressure, and flow rates.

The reactor was built as a part of the present research program and the effect of temperature and oxygen concentration on the product distribution was investigated.





### LITERATURE SURVEY

The oxidation of hydrocarbons may be divided into three distinct systems: slow oxidation for reaction temperatures between 200 and 600°C, catalytic oxidation, and explosive oxidation at high temperatures. Explosive oxidation is not considered in this survey as it is not applicable due to its immeasurably fast reaction rate. Catalytic oxidation, in most cases an industrial process, is discussed only to the extent that it has been used to study the reaction mechanism of hydrocarbon oxidation.

Zeelenberg and Bickel(46) state that slow oxidation of hydrocarbons is often characterized by an induction period, varying from seconds to hours, during which the conversion is very small. The reactions during this stage are important as they form intermediate products which lead to the primary oxidation process. The reaction rate then increases rapidly to form products including acids, aldehydes, ketones, peroxides, and carbon oxides.

Under certain conditions in the reaction between hydrocarbons and oxygen a "cool flame" front occurs. According to Minkoff and Tipper(26) the "cool flame" has the characteristics of an explosive reaction but the maximum temperature is less than 150°C above the initiation temperature and only a small portion of the reactants is consumed. Products formed include aldehydes and peroxides.



Fundamental reviews of hydrocarbon oxidation are given in books by Brooks(5), Goldstein(13), Jost and Kroft(17), Lewis and von Elbe(21), Marek and Hahn(24), Minkoff and Tipper(26), and Shtern(39).

#### A. Experimental Investigations and Fundamental Results

Experimental investigations of the partial oxidation of hydrocarbons have been carried out by a number of research workers. These investigations may be divided into several categories including the effect of reaction variables, surfaces, and catalysts on the reaction, the use of specialized equipment, and the method of product analysis. Recent work in each category will be discussed with emphasis on experiments relating to the vapor phase oxidation of n-butane.

##### 1. Reaction Variables:

Duthie(11), Dalla Lana(9,33), and Musgrove(27) carried out experiments to determine the effect of temperature, pressure, residence time, and inlet gas composition on the partial oxidation of n-butane in the vapor phase at the University of Alberta between 1950 and 1960. Duthie and Dalla Lana used a spiral reactor 24 feet long, made from  $\frac{1}{4}$  inch, Type 304 stainless steel pipe, and immersed in boiling Aroclor for temperature control. Musgrove used a variable length reactor of  $\frac{1}{4}$  inch stainless steel pipe with Aroclor as the heat transfer medium.





Duthie(11) designed and built the spiral reactor and carried out initial investigation of the variation of the reaction products with residence time. Dalla Lana(9,33) continued the work and studied the effect of pressure, inlet gas composition and residence time on the oxidation of n-butane. Optimum conditions for the spiral reactor were a pressure between 120 and 140 psia, a residence time of 1.2 to 1.8 seconds, and inlet n-butane and oxygen compositions between 4 and 5 mole per cent with a temperature of 725°F. These conditions gave 20 per cent conversion of the n-butane with about half of the carbon reacted going to useful products. The induction period, as indicated by the temperature profile, was in the order of 0.5 to 1.0 seconds.

Musgrove(27) investigated the effect of temperature and residence time on the reaction. The reactor was constructed by interconnecting a series of U-tubes in order to permit a choice of inlets with a fixed outlet. The residence time, for a constant mass velocity, was determined by the inlet point.

No reaction was observed at 675°F and only slight reaction at 700°F. The reaction rate increased rapidly between 700 and 725°F with a corresponding decrease in induction period. Above 725°F the rate increased only slightly and the reaction tended to go to carbon oxides.

Very little reaction occurred during the first 0.3 seconds at 725°F when the effect of residence time was studied. The reaction was very rapid between 0.6 and 0.7 seconds during



which time reactants were consumed. Following the period of very fast reaction, the rate decreased and very little reaction took place. By varying the mass velocity at constant residence time and temperature, Musgrove(27) found that the induction period decreased with decreasing mass velocity.

Steitz and co-workers(44), using a glass reactor with a length to diameter ratio of two and a volume of 415 c.c. at temperatures between 240 and 350°C and residence times between 3 and 793 seconds found similar results. Decreasing temperatures caused a decrease in overall reaction but an increase in carbon selectivity to chemicals and a decrease in carbon selectivity to hydrocarbons and carbon oxides. Optimum conditions of 270°C and a residence time of 40 seconds gave a carbon selectivity to chemicals of 80 per cent.

Furman and co-workers(12) studied the gas phase oxidation of n-butane at temperatures ranging from 325 to 375°C and pressure of 5 to 15 atmospheres and found that, by raising the pressure, the yield of oxygenated products, especially methanol, increased. By lowering the reaction temperature from 400°C to 350°C, they increased the efficiency of utilization of the n-butane.

With the debut of gas chromatography it has become possible to study the induction period of the partial oxidation reactions experimentally. In the induction period, the concentration of products is very low and accurate analysis previously was impossible.





Zeelenberg and Bickel(46), using a static system, varied the reaction temperature and the ratio of i-butane and oxygen in order to study the induction period of the i-butane oxidation. The induction period varied between 2 and 120 minutes and could be divided into stages. In the first stage, observed only for the formation of i-butene, products formed as a linear function of residence time. The second stage covered most of the induction period and concentrations of products increased as much as 100-fold. Products identified included i-butene, acetone, i-butene oxide, propionaldehyde, i-butyl alcohol, propylene, acetaldehyde, propylene oxide and methanol. The final stage in the oxidation process was the period from the end of the induction period onwards.

Neiman and Feklisov(28) in their study of the oxidation of Butane-1-C<sup>14</sup>, presented a relationship for the induction period of n-butane in a static system as:

$$\tau (P - P_O)^{1.2} e^{-22000/T} = \text{constant} \quad (1)$$

where

$\tau$  = induction period

$P_O$  = initial pressure in the static system

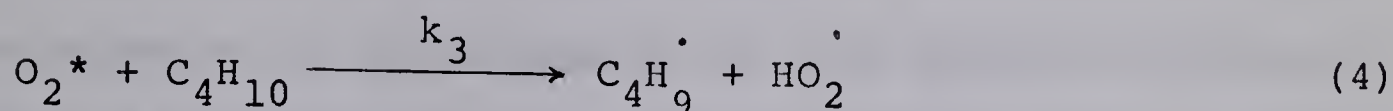
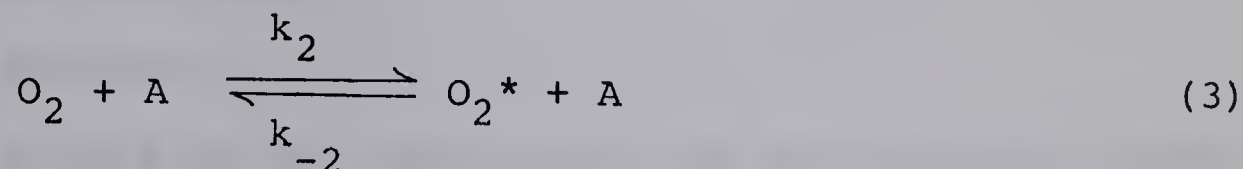
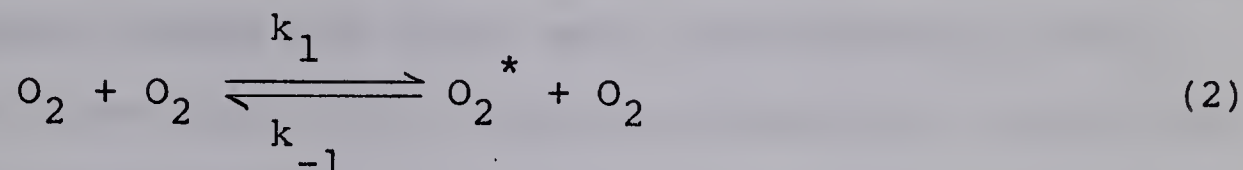
$P$  = final system pressure

$T$  = reaction temperature

Skrivan(40,41) studied the initiation reactions for the partial oxidation of n-butane in a flow reactor 1-1/4 inches in length and with a volume of 22.7 c.c. An initiation step involving activated oxygen molecules formed by oxygen-oxygen



collisions was proposed. The activated oxygen molecule reacted with the butane molecule to form butyl and hydroxyl radicals.



The reaction temperature was varied between 275 and 300°C with a contact time between 1 and 10 seconds. Initial oxygen concentrations were 20 and 40 mole per cent.

At 20 per cent inlet oxygen concentration, the n-butane conversion increased with residence time to a constant value of 10 per cent at approximately 3 seconds for temperatures below 350°C. At 350°C, the conversion increased with residence time but with increased formation of carbon oxides. At 40 per cent inlet oxygen concentration, the n-butane conversion reached a maximum at a 1-second contact time due to periodic "cool-flame" formation. This resulted in acceleration of reactions leading to the formation of hydrogen, methane, ethylene, and propylene. Maximum formation of these components occurred at a 1-second contact time because of the periodic "cool-flame" formation.

Carbon monoxide, carbon dioxide, and water formation all increased with residence time at each temperature level.



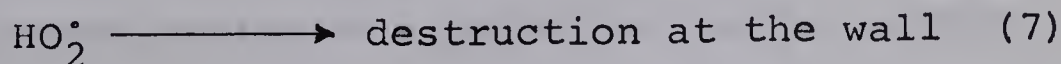
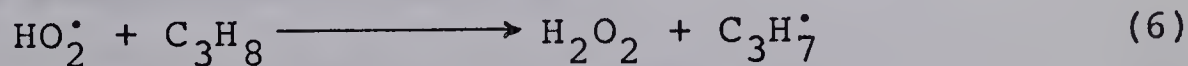
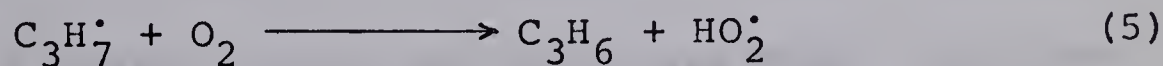


At temperatures of 275 and 300°C, carbon dioxide concentrations were negligible below a 1 second contact time. The concentrations of carbon oxides and water were approximately double that of the 20 per cent inlet oxygen concentration experiments for the 40 per cent runs.

## 2. Surface Effects:

The effect of the reactor wall on the products formed in the oxidation of hydrocarbons has been studied extensively. Appleby and co-workers(1) found that a pyrex reactor produced higher methane and lower ethane concentrations than a Pyrex reactor coated with KCl for the reaction between n-butane and oxygen in a static system. The appearance of peroxides in the pyrex reactor was also noted.

Satterfield and Reid(36) used a borosilicate glass reactor uncoated, coated with KCl, and coated with B<sub>2</sub>O<sub>3</sub> along with a stainless steel and alundum reactor to study surface effects on the partial oxidation of propane. The important reactions were given as:





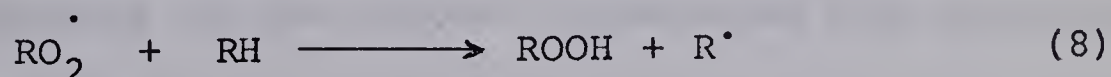


At 375°C, the ratio of hydrogen peroxide to propylene was independent of residence time only in the borosilicate tube but at 475°C the ratio dropped rapidly because of wall destruction of the peroxide radical. No hydrogen peroxide was identified in the products obtained from the Stainless Steel reactor at any temperature due to surface decomposition.

Norikov and co-workers(30) studied the effect of quartz, KCl coated quartz, and Stainless Steel reactor surfaces on the partial oxidation of n-butane at 260°C in reactors 5 centimeters in diameter and 18 centimeters long. Similar products were formed, with the exception of propionaldehyde, but in different proportions for the various reactors. A typical analysis is shown for each reactor with all figures being a percentage of oxygenated products.

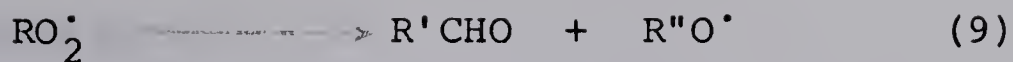
	Quartz	Quartz & KCl	Stainless Steel
Propionaldehyde	5.2	0.0	0.0
Acetaldehyde	40.3	33.6	27.5
Acetone	12.0	41.4	58.3
Hydroperoxides	42.5	25.0	14.5

The KCl coated quartz and Stainless Steel reactors decreased the bimolecular interaction



and favoured the isomerization and decomposition to acetone and acetaldehyde, as indicated below, stopping the decomposition to propionaldehyde.





Blyumberg and co-workers(3) obtained similar results in their oxidation of liquid n-butane in glass and stainless steel reactors at 150°C and 50 atmospheres. The glass reactor gave higher hydroperoxides and transformation product and lower decomposition product compositions. The main transformation products were methyl ethyl ketone and sec-butanol.

Chernesky and Bardwell(7) used a silica reactor with various coatings to study the surface effects on n-butane oxidation. They found that the  $\text{HO}_2^\cdot$  radical was important in the surface reaction and determined the extent of the reaction depending on the degree to which it was destroyed. PbO on the silica reactor acted as an effective inhibitor and stopped the reaction completely unless the temperature was raised substantially.

Skrivan(40) showed that no reaction between n-butane and oxygen occurred in a reactor filled with small stainless steel chips at temperatures up to 420°C, compared to a temperature range of 270 to 350°C for the empty reactor. The high surface area inhibited the reaction by destroying the  $\text{HO}_2^\cdot$  and  $\text{C}_4\text{H}_9^\cdot$  radicals as they formed. However, stainless steel chips in the entrance section to the reactor eliminated the induction period for the reaction.





### 3. Catalytic Effects:

The catalytic effects that are of interest are the action of homogeneous additives on product distribution and overall reaction of the hydrocarbons. Shtern(39) reported that carbon dioxide added to the reaction stream caused an increase in the n-butane conversion and the aldehydes formed. Hydrogen, helium, and argon also accelerated the oxidation of n-butane by increasing the difficulty of diffusion of the active centers to the wall which decreased the chain breaking. This caused an increase of intermediates in the gas phase which enabled the rate of initiation of active centers to increase by means of degenerate branching.

Dardin and Albright(10) used ozone in the oxygen stream in their study of the partial oxidation of propane and found that the reaction temperature required to give conversions of oxygen and propane decreased as the ozone concentration increased from 0 to 4 mole per cent of the inlet oxygen stream. The ozone had little effect on the product distribution.

Slavinskaya and co-workers(42) reacted oxygen and n-butane in the presence of ozone in a quartz reactor at temperatures between 65 and 300°C. The addition of ozone gave higher n-butane conversion and increased the yield of aldehydes. Shtern(39) indicated that the increase of hydrocarbon conversion in the presence of ozone occurred by the mechanism of the decomposition of ozone to give oxygen atoms. The oxygen atoms reacted with the hydrocarbon to initiate the chain reaction.





#### 4. Specialized Equipment:

The partial oxidation of hydrocarbons has been studied by research workers in equipment that deserves individual description. Such equipment includes a raining solids reactor, a motorized engine, and a cold-hot annular tube reactor.

Jones and Fenske(16) used a raining solids reactor with multiple oxygen injection points in their study of the partial oxidation of several hydrocarbons. The raining solids, between 125 and 300 microns in diameter and at rates of 5 to 10 pounds of solids per pound of feed, provided temperature control in the reaction zone to within 10 to 20°C of the desired reaction temperature. Too high a solids concentration decreased the reaction due to the inhibiting effect of the excess surface on the free radical reactions. At 400°C and 50 psig, oxidation of n-butane gave a high concentration of oxygenated products while, at atmospheric pressure, olefins predominated. The oxygenated products consisted of C<sub>1</sub> to C<sub>3</sub> aldehydes and alcohols while the olefins were largely butenes with minor amounts of ethylene and propylene.

Jones and co-workers(15) continued work with the raining solids reactor and obtained optimum reaction conditions for n-butane oxidation at 375°C and high solids rate with a 7 second contact time. These conditions gave maximum conversion with a high yield of oxygenated products. An increase in residence time increased carbon dioxide production at the expense of oxygenated products and olefins.



Boegel and co-workers(4) used a motored engine reactor with a compression ratio that could be varied up to 32 to 1. The advantage of a motored engine was that the cycle operation gave high temperatures and pressures for only a very short period of time. This permitted the reactions to be initiated and then quenched at any stage by the proper selection of reaction variables. Thermal cracking and oxidation of n-pentane took place at peak temperatures in excess of 1000°F. Conversion of n-pentane to oxygenated products was limited but the thermal cracking was extensive.

Oberdorfer and Winch(31) studied the oxidation of methane in a motored engine reactor with a compression ratio of 40 to 1. Methanol, formaldehyde, and formic acid were the chief products formed. Carbon monoxide and hydrogen were also formed in an amount approximately equal to the total oxygenated products at peak temperatures up to 1400°F.

Gudkov(14) employed an annular tube reactor in the study of methane and propane oxidation. The outer wall of the annulus was heated to 600 to 700°C and the inner wall of the annulus was cooled. Water passed up through the inner tube to keep the wall cool and a water film also flowed down the outer surface. Diffusion processes played an important part in the reaction as intermediates, formaldehyde and methanol, diffused into the water film and were removed from the reactor before they reacted further. The temperature in the annular space was more or less stable with the major temperature





gradients being in the boundary layers at the walls. Methane and propane oxidation in the cold-hot reactor produced formaldehyde concentration 5 to 6 times higher for methane and 2 to 3 times higher for propane than in any ordinary tubular reactor at the same conditions.

#### 5. Product Analysis:

Prior to the debut of gas chromatography as a method for the quantitative analysis of complex product mixtures a variety of chemical and physical analyses had been used.. One technique was fractional distillation of the liquid product and Orsat analysis of the gas samples by Duthie(11). Dalla Lana(9) and Musgrove(27) analysed the liquid product by mass spectrometer and the gas samples by Orsat analysis. A combination of chemical, polarographic, and mass spectrometric methods were employed by Oberdorfer and Winch(31).

Gas chromatography provides a more accurate analysis than any of the previous methods, especially for components having a very low concentration. Skrivan(40), Kalvinskas(18), Sandler and Beech(35), and Kyryacos and co-workers(20) have all used gas chromatographic procedures to analyse products formed in the partial oxidation of hydrocarbons.

#### B. Reaction Mechanism and Rate Expressions

During the early research on hydrocarbon oxidation several chemical schemes were put forward for the mechanism of this reaction. They have been discussed in detail by

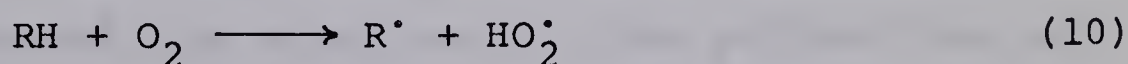




Dalla Lana(9), Kalvinskas(18), and Shtern(39) and will not be discussed further in this survey.

The most recent mechanism, a free radical-chain scheme, involves the formation of intermediate peroxide and hydrocarbon radicals. Benson(2) describes a chain reaction as the sum of a number of chain steps to yield the overall reaction. Reactants are consumed and products produced but the concentration of intermediates which propagate the reaction is controlled by initiation and termination steps. The number of overall reactions between initiation and termination is the chain length.

The chain initiation step for the oxidation of hydrocarbons is presented by Shtern(39) and Appleby and co-workers(1) as the reaction between a hydrocarbon molecule and an activated oxygen molecule to form radicals, as shown below:



Skrivan(40) used the activated oxygen molecule theory in the partial oxidation of n-butane to describe the initiation reaction and postulated that the activated oxygen molecules were formed in the collisions with other molecules. Equations (2) and (3) represent the formation of activated oxygen molecules by collision with other oxygen molecules and any other molecule A. Equation (4) is the reaction between the activated oxygen molecule and the butane molecule.

The rate of conversion of butane is given, according to Skrivan, from equation (4) as:



$$\frac{dx_B}{dt} = - k_3 x_{O_2}^* x_B \quad (11)$$

$$= - \frac{k_3 k_1 x_B x_{O_2}^2}{k_{-1} x_{O_2} + k_3 x_B} \quad (12)$$

If  $k_{-1} x_{O_2}$  is considered negligible compared to  $k_3 x_B$ ,

$$\frac{dx_B}{dt} = - k_1 x_{O_2}^2 \quad (13)$$

where

$x_B$  = butane concentration in mole fraction

$x_{O_2}$  = oxygen concentration in mole fraction

$t$  = time

$k_1$  = forward rate constant of reaction (2).

To check the proposed rate equation, Skrivan plotted the rate of butane conversion versus the oxygen concentration on a log-log plot which gave a linear relationship with a slope of 2.2. This slope compared favorably with the theoretical slope of 2 from equation (13). As a further check of the rate equation, the rate of butane conversion was plotted against the second power of the oxygen concentration at constant temperature. The plot gave a linear relationship with a slope equal to the rate constant and passed through the origin.

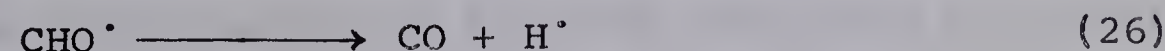
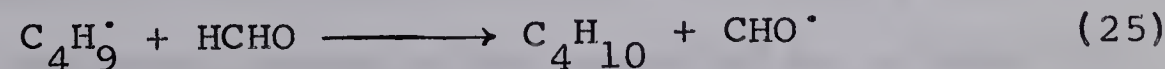
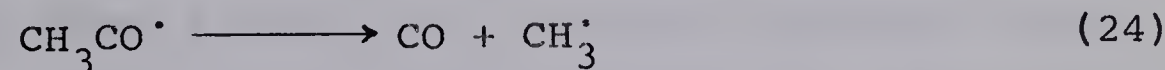
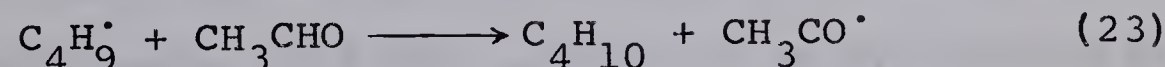
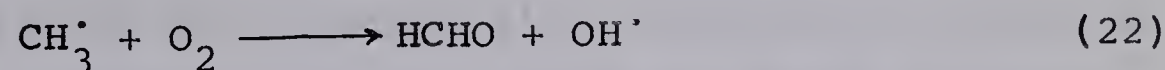
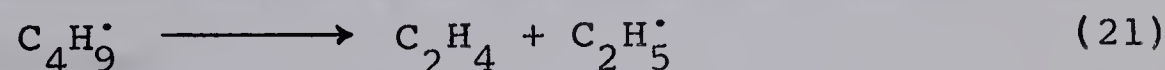
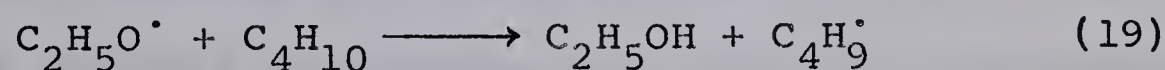
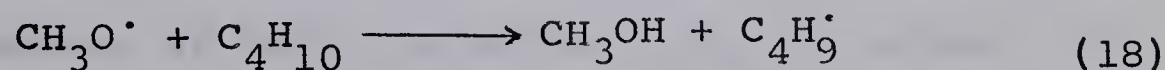
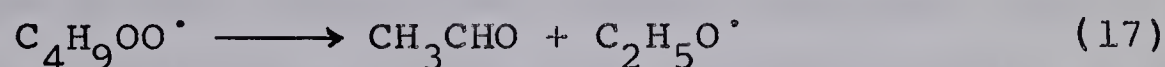
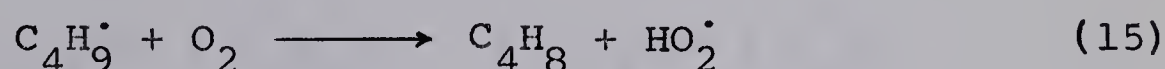
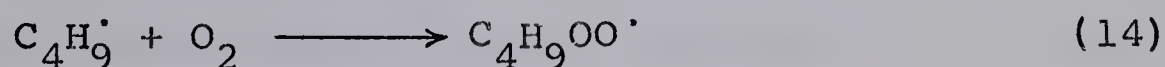
Skrivan(40) proposed a set of twenty-two equations to account for the major components identified by gas chromatography. The components were mainly in three categories,



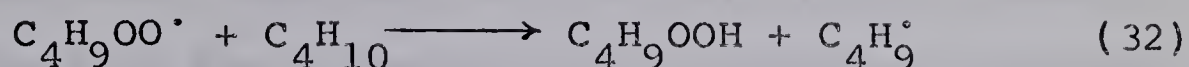
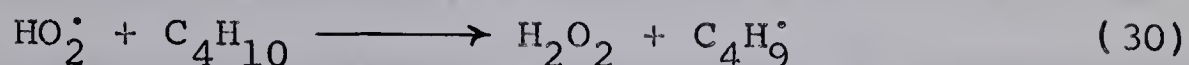
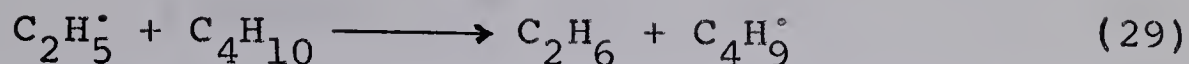
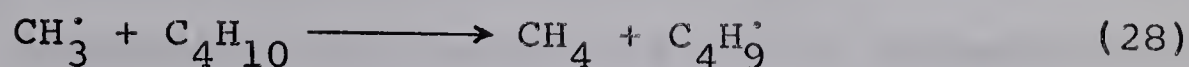




namely, butenes, cracking products, and oxygenated compounds. The reactions all depend either directly or indirectly on the path of the butyl radical. The three initiating reactions have been given in equations (2), (3), and (4). The remaining equations, mainly chain propagating equations, are as follows:

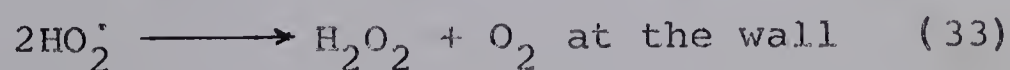






The work of Norikov and Blyumberg(29) supports this reaction scheme as they identified isobutyl peroxide radicals in the oxidation of i-butane. Cartlidge and Tipper(6) found appreciable amounts of butyl peroxide,  $\text{C}_4\text{H}_9\text{OOH}$ , present as well as hydrogen peroxide in a glass reactor at 315 to 345°C. Zeelenberg(45) oxidized neo-pentane and identified neo-pentyl radicals. He described the termination step as the reaction between the peroxide radicals and hydrocarbon radicals to form alkyl peroxides.

Satterfield and co-workers(38) studied the oxidation of propane at temperatures between 350 and 475°C and their reaction products agree with the scheme set up by Skrivan(40). In a spherical glass reactor with reactants entering tangentially and products being removed at the center, a high concentration of hydrogen peroxide was reported as a means of supporting the formation of the peroxide according to reaction (6) rather than by the reaction



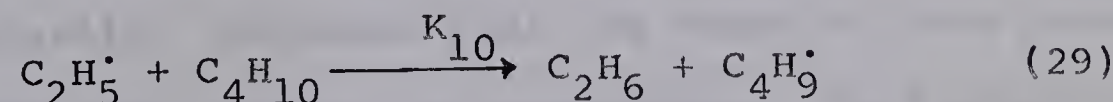
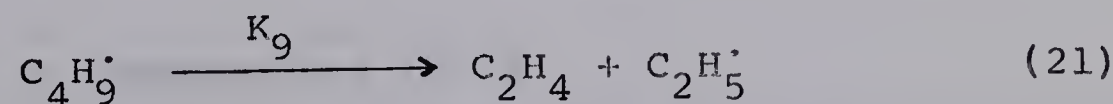
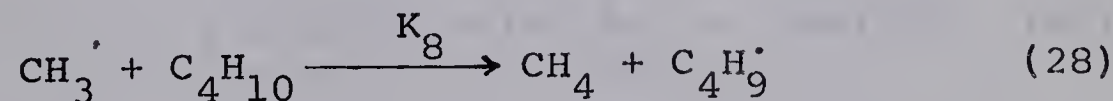
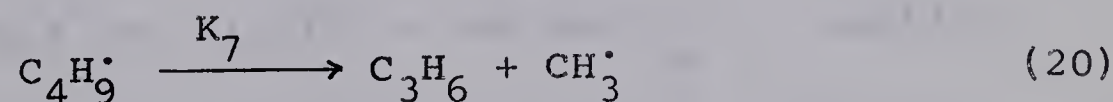
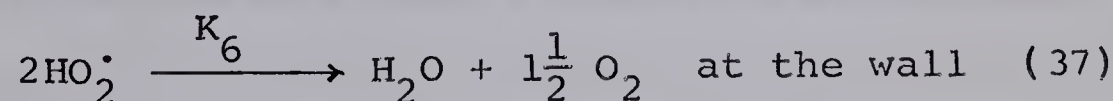
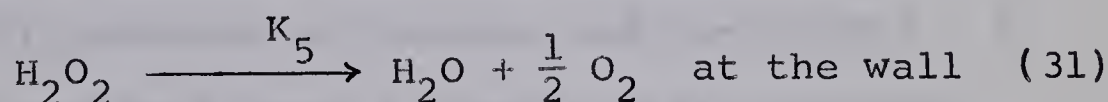
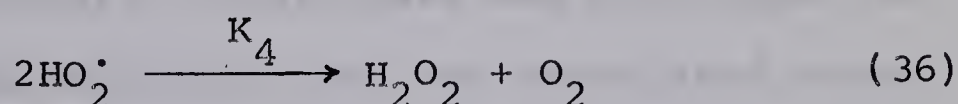
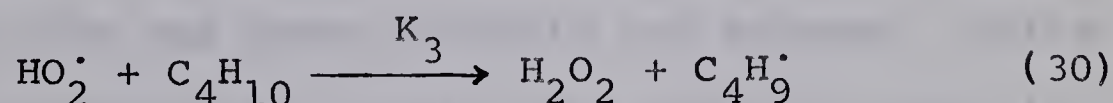
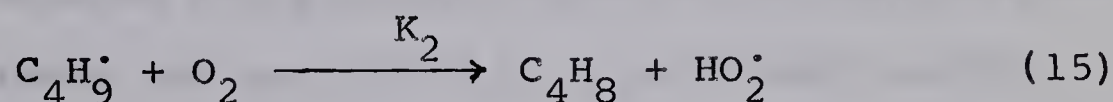
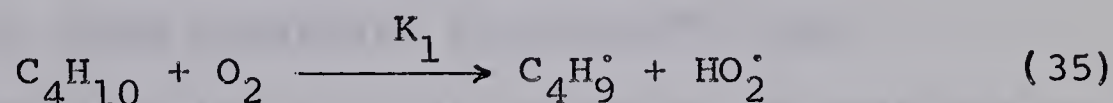




The disappearance of propionaldehyde at high temperatures is explained by Satterfield and co-workers as the decomposition



Appleby and co-workers(1) outlined a set of ten reactions for the partial oxidation of n-butane at temperatures around 500°C. At these temperatures the free radical reactions of hydrocarbons were important and the only liquid product was water formed by the decomposition of hydrogen peroxide. The reactions, given below, indicate the absence of carbon oxides and hydrogen.







Appleby and co-workers(1) derived a rate expression from the above equations, which is given as:

$$-\frac{d(C_4H_{10})}{dt} \approx \sqrt{2K_3} \sqrt{\frac{K_1}{K_4}} (C_4H_{10})^{3/2} (O_2)^{1/2} \quad (38)$$

or

$$-\frac{d(C_4H_{10})}{dt} = K(C_4H_{10})^{3/2} (O_2)^{1/2} \quad (39)$$

where

$C_4H_{10}$  = mole fraction of n-butane

$O_2$  = mole fraction of oxygen

$K$  = rate constant, lb.moles/ft.<sup>3</sup> min.

Kalvinskas(18) studied the partial oxidation of n-butane at temperatures between 360 and 760°C in a porcelain reactor. He analysed only the gas phase products and assumed, similar to Appleby and co-workers(1), that there was only water in the liquid phase. The oxidation data was correlated using the rate equation (39) proposed by Appleby and co-workers. A least squares fit of the data gave a reaction rate constant equation:

$$\begin{aligned} \log K = & -1.1797 - 746.647 \left( \frac{1}{T} - .00135 \right) \\ & + 1.25508 \times 10^7 \left( \frac{1}{T} - .00135 \right)^2 \end{aligned} \quad (40)$$

where

$T$  = temperature in °K

Kalvinskas(18) indicated that the reaction rate passed through a minimum with respect to temperature. This phenome-



non was noted before by Satterfield and co-workers(38) in the oxidation of propane and was discussed by Shtern(39). The decrease in reaction rate is due to a change in mechanism as the temperature increases. At low temperatures the reaction rate is high because of the importance of the peroxide radical reactions but at high temperatures the cracking reactions give the high reaction rate. At intermediate temperatures it is possible to obtain the situation in which the peroxide radical reactions have ceased to be important due to the instability while the cracking reactions have not become prominent because of too low a temperature. This results in a decreased reaction rate.

### C. Summary

As indicated by the discussion of literature published on the partial oxidation of hydrocarbons, much work has been done using both static and flow systems to describe the effect of reaction variables on the overall reaction and to determine the reaction mechanism. However, there is a shortage of information on the effect of residence time on the reaction and on reactions occurring during the initiation period.

In the static systems used by Zeelenberg and Bickel(46), Appleby and co-workers(1), and others, the reaction between the hydrocarbon and oxygen took place for a certain period of time and was terminated by cooling the product gases below







reaction temperature. The length of time that the reactants were in the reaction vessel governed the residence time. A sample taken from the reaction mixture after the reaction was stopped was analysed in order to determine the product distribution. To study the effect of residence time, a number of experiments were necessary and, as a result, any variations in initial temperature and gas compositions caused differences in product distribution that were not due to the effect of residence time.

For flow systems, two methods were used to study the partial oxidation of hydrocarbons. Dalla Lana(9) and Skrivan(40) were among the group of research workers that used a reactor of constant length and varied the flow rate through the reactor to obtain different residence times. With this type of a system, the effect of mass velocity on the reaction interfered with the effect of residence time. Musgrove(27) and Kalvinskis(18), along with other workers, varied the residence time in their equipment by varying the reactor length. This technique provided information for variable residence times at a constant mass velocity but separate runs were required for each residence time.

In most flow systems, sampling of the product stream took place at the reactor exit after the reaction gases had been cooled by water injection and over a considerable period of time. The water injection provided rapid quenching but



created inaccuracies in the liquid product analysis due to dilution. Sampling over a long period of time gave average values for product distribution but any instabilities in the system during the sampling period caused errors.

The work of Jones and Fenske(16) and Jones and co-workers(15) with the raining solids reactor was important as it provided a method of temperature control in the reaction zone. If the exothermic heat of reaction is not removed rapidly, the reaction temperature increases by as much as 100 to 300°F and a different set of reactions becomes important. Use of the raining solids maintained reaction temperatures within 10 to 20°C of the inlet temperature without significantly inhibiting the reaction.

The free radical-chain mechanisms proposed by Skri-  
van(40) and Appleby and co-workers(1) differ, depending on the temperature range involved. The mechanism used by Skri-  
van for temperature between 275 and 350°C described the formation of aldehydes, alcohols, peroxides, unsaturated and saturated hydrocarbons, water, and carbon monoxide. However, it failed to describe the formation of either carbon dioxide which was present in most product analyses or ketones which have been reported by Dalla Lana(9), Norikov and co-workers(30) and others.

The reaction scheme proposed by Appleby and co-workers(1) for temperatures near 500°C and used by Kalvinskis(18) for temperatures between 360 and 760°C predicted the formation





of unsaturated and saturated hydrocarbons, hydrogen peroxide, and water. It did not explain the formation of carbon oxides even though they were reported by both Appleby and co-workers and Kalvinskas. It neglected the formation of oxygenated products which are known to be present, especially at the lower temperatures used by Kalvinskas.





### SCOPE OF THIS INVESTIGATION

The overall scope of the study of the partial oxidation of n-butane, of which this is the first phase, is the investigation of the effect of reaction variables on product distribution and the examination of methods of temperature control in the reaction zone. The basic purpose of the study is to obtain information on the initiating reactions and reaction mechanism with the ultimate goal being a rate expression.

The initial step in the present program was the design and construction of a reactor that would be versatile and easily adaptable over a wide range of temperature, pressure, and flow conditions. Much of the versatility was included so that future work may be carried out without major equipment revision. A study of the equipment used by researchers in previous flow systems indicated several ways that the present equipment design could be improved. These improvements either eliminated or minimized variations in product distribution caused by effects other than the effect of the reaction variable to be studied.

The reactor was designed with five sample points along the reactor which permitted multiple sampling of each experimental run. Previous research workers sampled product gases at the exit only and had to make multiple runs with either different flow rates or different reactor lengths in order to



study the effect of residence time on the overall reaction. Product distribution differences were introduced, not only because of the effect of residence time which was desired, but also due to slight differences in the system parameters for the different runs and the effect of the flow rate through the reactor. The present reactor, with multiple sample points, eliminates the outside effects as each experimental run permits samples to be taken at five residence times.

Rapid sampling was incorporated into the design of the sampling system in order to minimize the effect of any fluctuations in the system during sampling. If a sample is collected over a considerable period of time, any fluctuations cause product composition variations and the sample obtained is an average one. Rapid sampling, in the order of 5 to 10 seconds per sample, decreases the possibility of any fluctuations occurring and allows resampling if any fluctuations in reaction conditions were noticed. Rapid sampling was only possible because a gas chromatograph was to be used for product analysis and only a small sample was required.

The control of all reaction variables, namely, temperature, pressure, and reactant flow rates, was accomplished by the use of either pneumatic or electronic control circuits. The use of the control circuits gave accurate control of the reaction variables, much more so than manual control. Furthermore, duplicate experimental runs could be made at exactly the same conditions in order to check reproducibility of







results.

Allowances were made in the design of equipment so that it could be adapted to many uses. Each major component, such as the feed system, the preheater, the reactor, and the exit section, is designed to be independent of all others to allow any one section to be changed without affecting the others. The basic design included pieces of equipment in the preheater and exit section to allow future modification of the system to study suspended solids flow in the gas stream as a means of temperature control. Extra coils are designed for the preheater in which the solid particles may be heated to the entrance temperature. The exit section design includes a cyclone separator and solids container for the removal and storage of the solids.

Initial evaluation of the equipment and investigation of the effect of inlet temperature and oxygen concentration on the partial oxidation reaction were the final steps in the present program. By choosing the correct residence time for the n-butane and air, it was possible to obtain product samples in the induction period, during the period of rapid reaction, and in the period following the rapid reaction when little reaction takes place. Analysis of the samples provided information on the course of the reaction and, ultimately, should lead to a better knowledge of the initiating and secondary reactions.



## EQUIPMENT AND OPERATING PROCEDURE

The experimental equipment, as represented in Figures 1 to 7 inclusive, consists mainly of the n-butane and air feed systems, the preheater, the reactor with its temperature measuring and product sampling equipment, the temperature control circuits, and the gas chromatograph for analysis of the product samples.

Figure 1, a schematic diagram, gives the overall layout of the equipment and instrumentation used to control the feed rates, the reactor pressure, and the preheater and reactor temperatures. Preheater and reactor details are shown in Figures 2 and 3, respectively. These Figures outline the n-butane and air preheater coils, the mixing section at the reactor entrance, and the reactor. Also shown are the location of thermocouples for temperature measurement and control in the preheater and reactor as well as the positioning of the sample lines along the reactor. Figure 4 locates the thermocouples, between any two electrical heaters, in the gas stream and reactor wall in relation to the sample lines and electrical heater leads. The electronic circuits, as depicted in Figures 5, 6 and 7, are used to control the preheater temperatures.





## A. Feed Systems

The n-butane is fed to the preheater as a liquid and the flow rate is controlled using a Foxboro Integral D/P Cell and Pneumatic Control Valve with a Foxboro Model 58 Universal Pneumatic Controller.

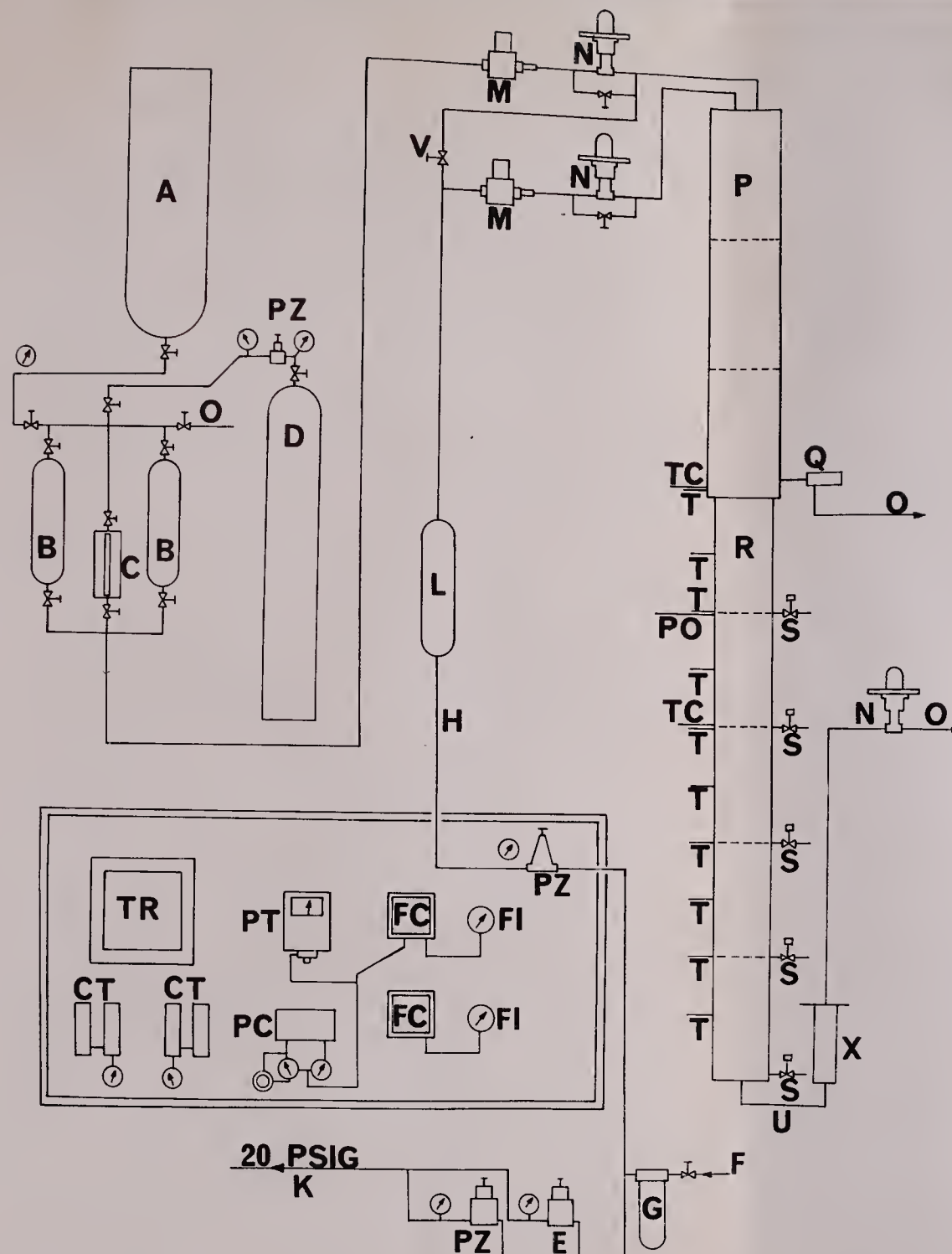
The n-butane is transferred from the storage tank, as shown in Figure 1, to the feed tanks by means of a pressure differential created by pressurizing the storage tank with nitrogen. The n-butane in the feed tanks is then pressurized with nitrogen and held at a constant pressure as the n-butane is fed to the preheater.

The n-butane feed tanks each have a volume of 0.288 cubic feet and are connected with 1/4 inch copper tubing in such a way that the feed may be drawn from one or both tanks simultaneously. With these connections, it is possible to be feeding from one feed tank while filling the second one from the n-butane storage tank. A sight gauge is incorporated in the feed tank system to allow checking of the n-butane liquid level in the feed tanks.

The liquid n-butane from the feed tanks flows through the Integral D/P Cell in which the flow rate is measured by the pressure drop in inches of water across the integral orifice. The Integral D/P Cell has an orifice diameter of 0.02 inches and a pressure difference range of 0 to 250 inches of water. The n-butane passes through the pneumatically operated







A BUTANE STORAGE  
 B BUTANE FEED TANK  
 C BUTANE LEVEL GAUGE  
 D NITROGEN CYLINDER  
 CT TEMPERATURE CONTROLLER  
 FC FLOW CONTROLLER  
 F AIR LINE  
 FI FLOW INDICATOR  
 G WATER TRAP  
 H PROCESS AIR  
 K INSTRUMENT AIR  
 L VOLUME TANK  
 M INTEGRAL D/P CELL AND CHECK VALVE  
 O EXIT & VENT LINES  
 P PREHEATER  
 PC PRESSURE CONTROLLER

PO PRESSURE TAP  
 PT PRESSURE TRANSMITTER  
 PZ PRESSURE REGULATOR  
 Q RELIEF VALVE  
 R REACTOR  
 S SAMPLE LINE  
 T RECORDING THERMOCOUPLE  
 TC CONTROL THERMOCOUPLE  
 TR TEMPERATURE RECORDER  
 U EXIT SECTION  
 X INLINE FILTER  
 V BYPASS VALVE  
 N CONTROL VALVE

FIGURE 1: SCHEMATIC LAYOUT OF EQUIPMENT. SCALE 1" = 2'



control valve and into the preheater coil. The control valve is a Foxboro Type V4 Needle Valve, body size 1/2 inch, with a needle size of 0.024 inches ( $C_v = 0.0052$ ). The  $C_v$  value of a control valve is defined as the number of U.S. gallons per minute of water discharged through the wide open valve with a 1 psi pressure drop across it.

The air to be fed to the preheater flows from a compressor operating at 90 psig. It passes through a trap to remove any entrained water (see Figure 1) and through a Cono-flow pressure regulator which regulates the air pressure to the D/P Cell and control valve. A volume tank, having a volume of 0.3 cubic feet, between the pressure regulator and the D/P Cell dampens any fluctuations in line pressure that pass through the regulator. A second volume tank, 0.1 cubic foot, acts to dampen any pressure fluctuations created by a sudden movement of the control valve before they reach the Integral D/P Cell. This volume tank is installed between the Integral D/P Cell and the control valve.

The Integral D/P Cell for the air has a 0.0595 inch diameter orifice and a pressure difference range set at 100 inches of water. The control valve is a Foxboro Type V4 Needle Valve, body size 1/2 inch, with a needle size of 1/8 inch ( $C_v = 0.07$ ).

The flow rates of the n-butane and air are each controlled with a Foxboro Model 58 Universal Pneumatic Controller







which receives a signal from the D/P Cell, compares it with the manual set point and sends a signal proportional to the error to the control valve to regulate the flow. The signal from each D/P Cell to the controller, which is a measure of the flow rate, is recorded on the recorder chart built into the Controller. In addition, the signal goes to a gauge with a square root dial which indicates the flow rate as a per cent of the maximum flow. With these gauges in the system, the n-butane and air flow rates may be checked without referring to the controller charts.

Instrument air for the flow control systems and the pressure control components is taken from the main air line immediately after the water trap, as indicated in Figure 1. This air stream passes through two Fisher Governor Company filter-regulators, in parallel operation, which remove any traces of water remaining in the air and reduce the pressure to 20 psig, the required instrument air pressure. Gauges on the filter-regulators indicate the instrument air line pressure.

Two features are incorporated in the feed system to insure safe operation of the equipment. Check valves are installed in both the n-butane and air lines immediately following the control valves to prevent any flow of gas or liquid mixtures back into the feed system. Also, the control valves on both feed lines operate in such a fashion that, in the event of failure of the instrument air, they automatically



close and stop all flow into the reactor. Other safety measures are taken and they will be described along with the part of the equipment containing the safety feature.

## B. Preheater

The preheater, as shown in Figure 2, contains the individual coils to preheat the n-butane and air, the electrical heaters, the n-butane and air mixing section just prior to the reactor entrance, and insulation to decrease heat losses to the surroundings.

The n-butane flows from the flow control valve to the preheater coil at the top of the preheater as a liquid and, as it flows downward, vaporizes and its temperature increases to the reactor entrance temperature. The air flows into a second coil at the preheater entrance and is heated while flowing through the coil.

The preheater coils are spiral coils made from Type 304 Stainless Steel tubing with a 0.375 inch outside diameter and a wall thickness of 0.065 inches. The spiral coils have a 6 inch pitch and an inside coil diameter of 2.875 inches. The n-butane coil is constructed from an 11 foot length of tubing to give 10 complete spirals with an overall length of 5 feet in the preheater and allowing 6 inches of tubing at each end for connections. The air coil is similar except that it has only 5 complete spirals. The preheater coils are supported by a 5 foot length of 2-1/2 inch mild steel pipe





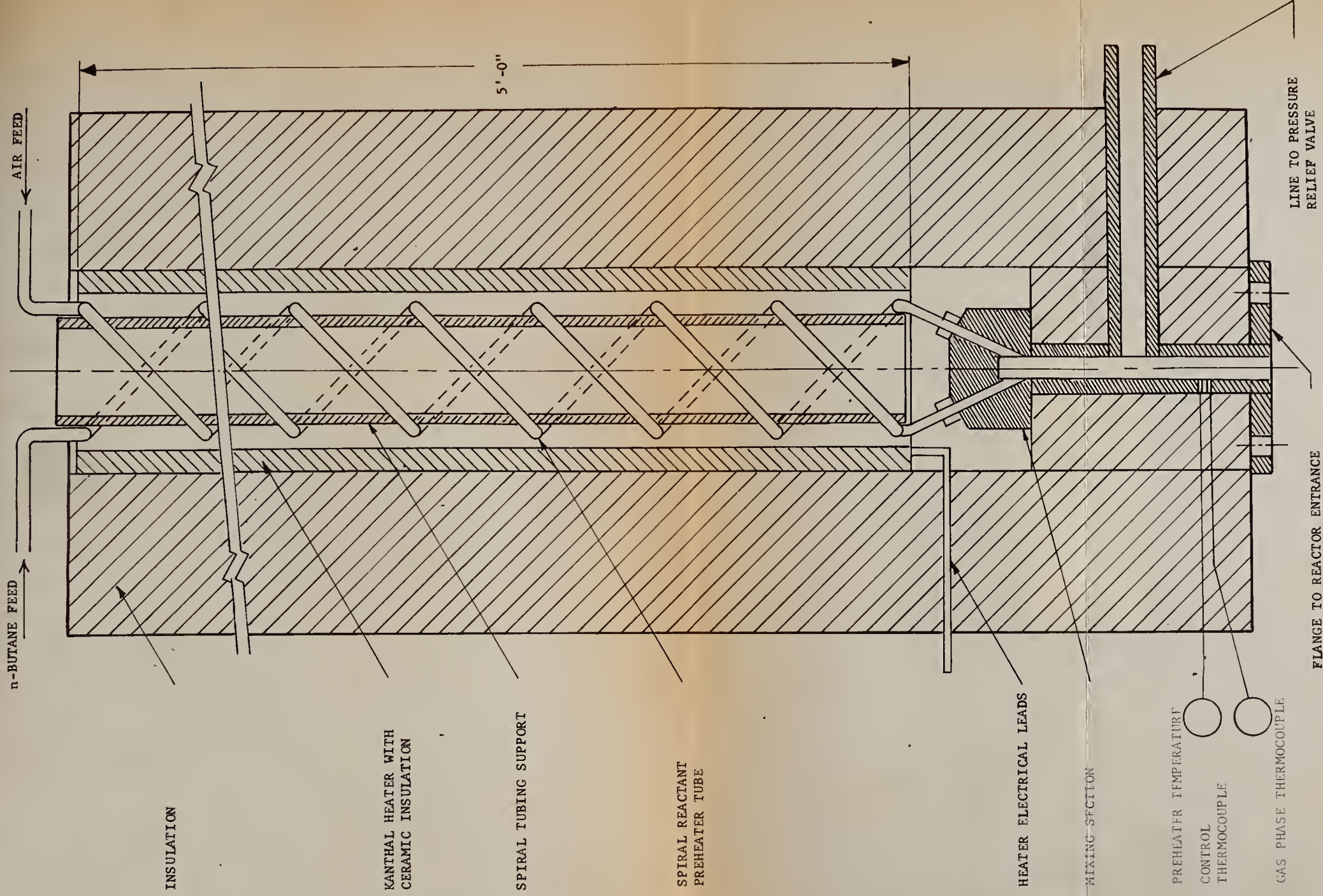


FIGURE 2: PREHEATER DETAIL. SCALE: 1" = 2.5"





inserted inside the coils. The n-butane coil extends all the way up the preheater and support pipe while the air coil, in the bottom part of the preheater, reaches only halfway up the preheater and support pipe. At this point the tubing passes through an opening in the support pipe wall and connects to a straight length of tubing to the top of the preheater.

Three cylindrical Kanthal heaters, Type REH 10-60, fit outside the preheater coils as the heat source. Each heater has a heating length of 19.70 inches, an inside diameter of 3.94 inches, and an outside diameter of 5.09 inches. The heaters are mounted vertically one above the other around the preheater coils with a gap of 0.3 inches between each to give a total heating height of 5 feet. The three heaters are connected in series, each heater having maximum rating of 2750 watts at 64 volts and 43 amperes, to produce a maximum heat load of 8250 watts at 192 volts and 43 amperes in the preheater.

The tubular element consists of a Kanthal A-1 alloy strip in the shape of a spiral. The individual turns of the spiral are insulated from each other with ceramic T-form separators. Thus, the turns can lie close to each other and produce a high concentration of heat and an equal temperature distribution inside the element. The T-separators are fixed to the outer side of the tubular element with a ceramic embedding material about 1/2 inch thick. The T-separators protrude beyond the Kanthal strip on the inner side of the tubular



element and prevent the preheater coils from touching and shorting the heater element.

Below the final heating element, the n-butane and air coils are connected to a common header, as indicated in Figure 2, with Swagelok Type 316 fittings. In the header the feed streams come together and mix as they flow through a 6-inch length of Type 316 Stainless Steel tubing, with an inside diameter of 0.625 inches to the reactor entrance.

Two thermocouples are inserted into the center of the gas stream through the tubing wall. One thermocouple measures and records the temperature of the gas in the mixing section and the second one acts as the measuring element for the preheater temperature control circuit.

A 3/4 inch Farris Safety-Relief Valve Type 2745/S4 is connected to the preheater mixing section with 3/4 inch Stainless Steel pipe fittings to guard against equipment failure in the event of a sudden increase in reactor pressure. The exit line from the Safety-Relief Valve connects directly to the steam ejector system used to vent all reaction products to the atmosphere. The Safety-Relief Valve, with a set of replacement compression springs, has a release pressure which is adjustable over a wide range. The release pressure is adjusted by interchanging compression springs.

The mixing section is insulated with asbestos tape 2 inches wide and 1/8 inch thick wrapped around the tubing and header to a thickness of 1 to 2 inches. A 4 inch thickness







of Johns-Manville Thermobestos pipe insulation fits outside the three Kanthal heaters and mixing section to minimize heat losses. Thermobestos pipe insulation is a calcium silicate insulation capable of withstanding temperatures to 1200°F and having a thermal conductivity of 0.045 BTU/hr.ft<sup>2</sup> °F/ft at an average temperature of 600°F.

### C. Reactor

The n-butane and air stream flows from the preheater into the reactor. Thermocouples in the gas stream and reactor wall measure gas and wall temperature profiles. Sample lines connect to sample bombs at various points along the reactor to allow sampling of the reacting gas stream.

The reactor is a 9 foot length of Type 316L Stainless Steel tubing with an inside and outside diameter of 0.625 and 1.25 inches, respectively. The heavy walled tubing is used to facilitate the installation of thermocouples and sample lines in the gas stream. Although at room temperature the reactor is 9 feet long, at reaction temperatures it increases by approximately 1 inch due to thermal expansion of the Stainless Steel tubing.

A flow nozzle in the reactor entrance, as shown in Figure 3, insures complete mixing of the reactant stream from the preheater. The nozzle has an entrance diameter of 0.625 inches which is the same as the reactor inside diameter, a throat diameter of 0.250 inches, and a downstream diameter



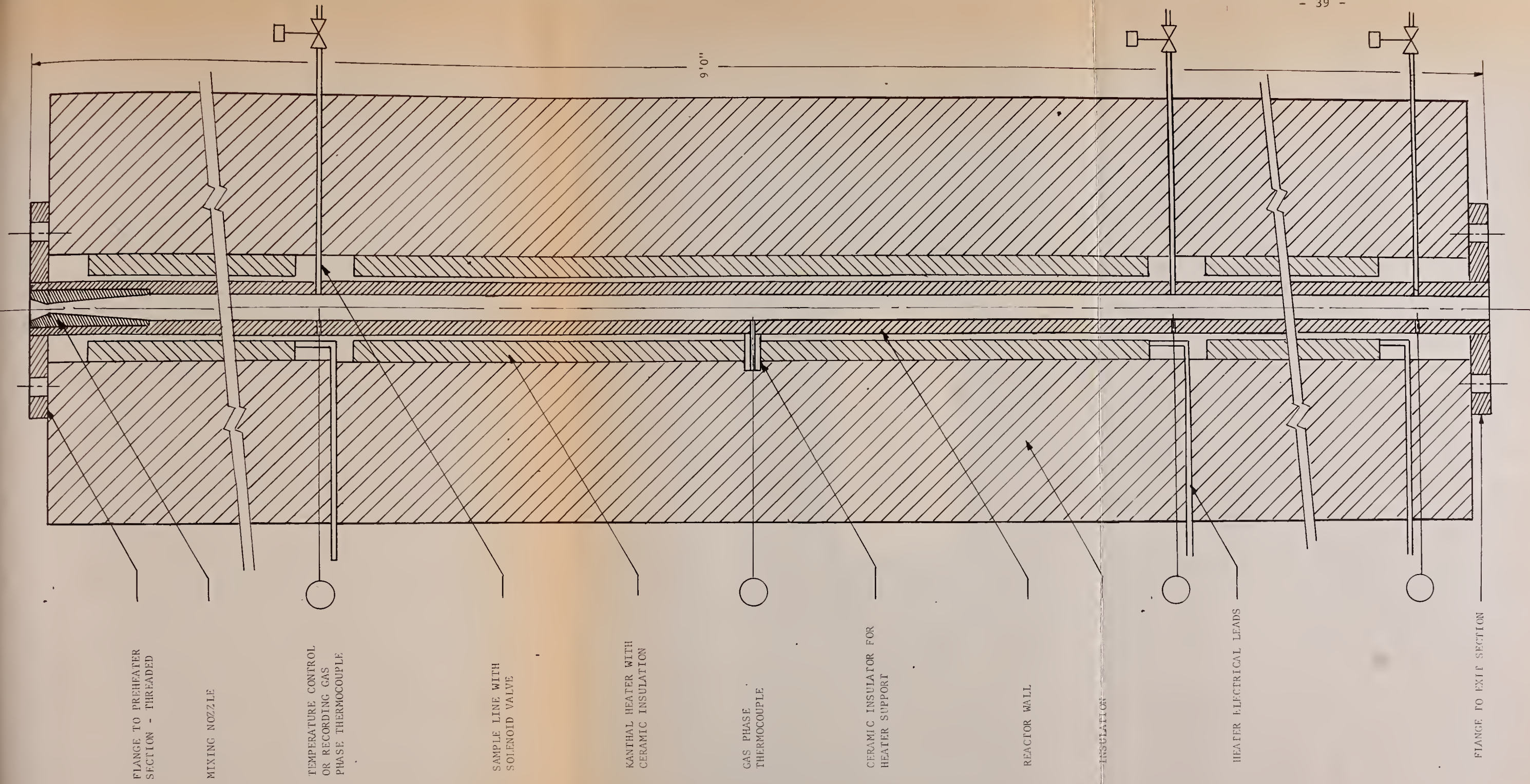


FIGURE 3: REACTOR DETAIL. SCALE: ONE-HALF







of 0.625 inches, to coincide with the reactor wall. The convergent upstream angle in the nozzle is 20 degrees and the divergent downstream angle is  $4\frac{3}{4}$  degrees which gives the nozzle an overall length of 3 inches. Transitions between the convergent section, the throat, and the divergent section are slightly rounded to remove any sharp edges.

The product gases leave the reactor through a  $1\frac{1}{2}$  inch Type 304 Stainless Steel pipe, pass through an in-line filter and a pressure control valve to be vented, through a steam ejector, to the atmosphere. The in-line filter is installed in the line to remove any solid particles that could plug or damage the pressure control valve. The filter element is a Selas Micro-Porous Porcelain Filter Candle Type FD128 which is contained in a Stainless Steel body. The filter candle is  $8\frac{1}{4}$  inches in length with an outside diameter and wall thickness of  $1\frac{1}{2}$  inches and  $\frac{1}{8}$  inch, respectively. The filter candle has an average pore diameter of 20 microns and a porosity of 40 per cent.

Five cylindrical Kanthal heaters, Type REH 4-60, fit outside the reactor tube. The heaters are similar to those used in the preheat section except that their sizes and maximum ratings differ. Each heater has a heating length of 19.70 inches, an inside diameter of 1.57 inches, and an outside diameter of 2.58 inches. The heaters are mounted with a space of 1.3 inches between them to allow room for the insertion of thermocouples and sample lines into the gas



stream and reactor wall. A distance of 1.5 inches is allowed from the reactor entrance to the top of the uppermost heater so that the reactor entrance flange can be screwed into place. The base of the bottom heater is 2.8 inches from the reactor exit. This space provides for the electrical heater leads of the last heater, the thermocouples and sample lines, and the flange on the reactor exit. Each heater has a small hole through the ceramic embedding material at its mid point so that thermocouples can be placed in the gas stream. The five Kanthal heaters are connected in series to give a maximum heat load of 6750 watts at 150 volts and 45 amperes.

The spaces between the heaters are wrapped with asbestos tape as insulation to give a diameter approximately equal to the heater size. A 4 inch thickness of Thermobestos pipe insulation fits outside the heaters and asbestos tape to cut down the heat losses. All thermocouples and sample lines pass through small openings in the insulation.

The reactor pressure is controlled by a Foxboro Model 58 P4 Pneumatic Controller which operates a control valve in the exit line to the steam ejector. A 3/16 inch Stainless Steel tube leads from a pressure tap below the uppermost reactor heater to a Foxboro M/44 Pressure Transmitter which measures the pressure and sends a pneumatic signal to the controller. This pneumatic signal is transmitted to the n-butane flow recorder where it is recorded on the same chart as the n-butane flow rate. The pressure controller adjusts





the position of the pressure control valve to maintain the reactor pressure at a value corresponding to the set point pressure. The control valve is a Foxboro Type V4 Needle Valve, body size 1/2 inch, with a needle size of 3/16 inches ( $C_v = 0.28$ ). The pressure control system operates so that, in the event of failure of the instrument air, the control valve opens wide and prevents the build up of reactor pressure.

The temperature of the reacting gas stream is measured using thermocouples inserted into the center of the gas stream through the reactor wall. There are ten thermocouples in the gas stream located at the mid point and below each of the five reactor heaters. The top thermocouple in the reactor is located 11.4 inches below the entrance and the remaining nine are spaced at 10.5 inch intervals. Five thermocouples are embedded in the reactor wall at points revolved 180 degrees from the gas stream thermocouples below each heater, as shown in Figure 4, to measure the wall temperature. Below the second heater from the top an additional thermocouple in the gas stream acts as the measuring element for the reactor temperature control circuit.

All thermocouples, except the two control thermocouples in the preheater and reactor, are connected to a Leeds and Northrup Speedomax G Millivolt Recorder. The recorder is a sixteen point recorder with variable range and zero. All sixteen recorder channels are used to record the ten gas phase and five wall temperatures in the reactor and



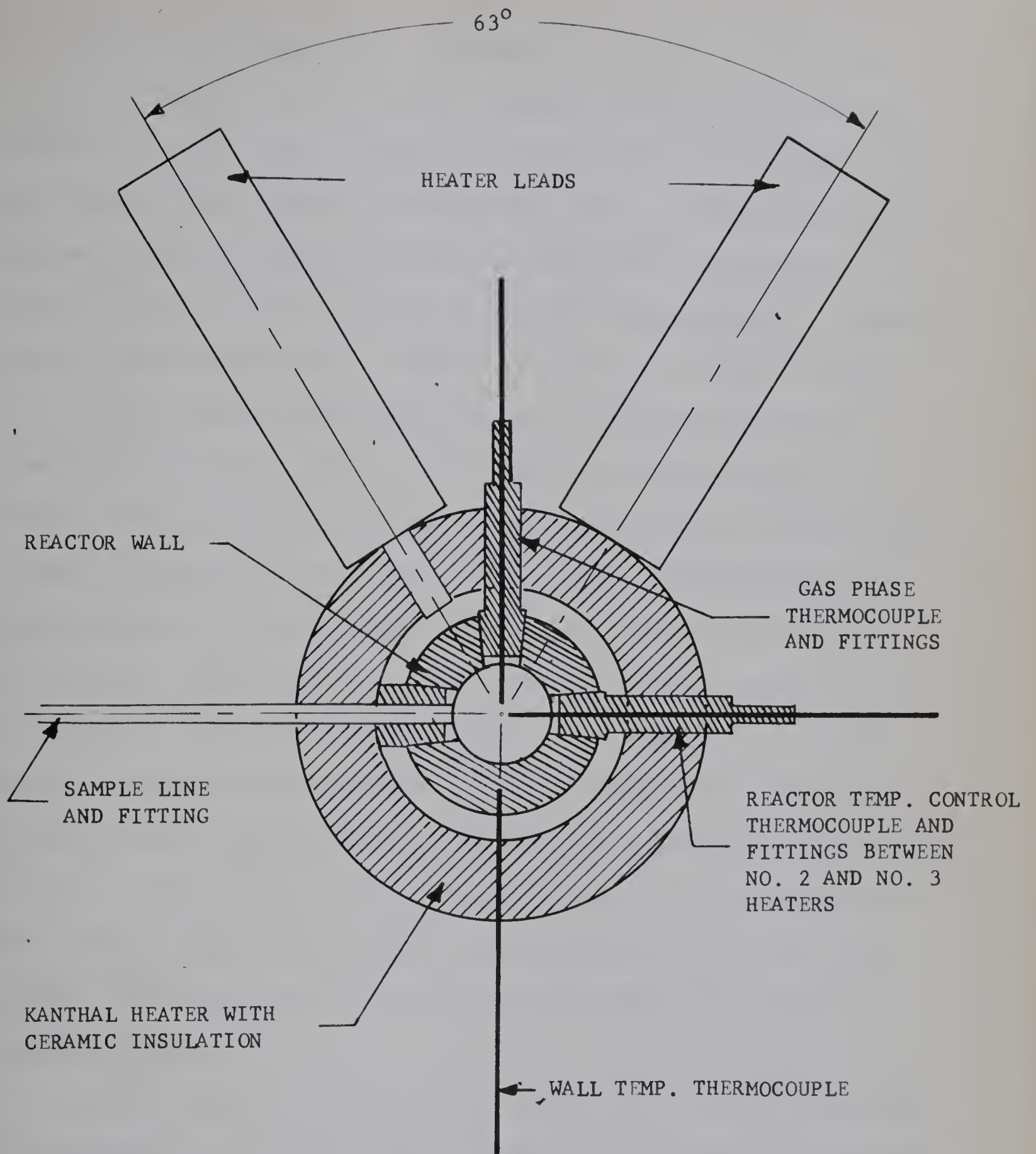


FIGURE 4: THERMOCOUPLE AND SAMPLE LINE  
LOCATION BETWEEN REACTOR HEATERS. FULL SCALE





the preheater temperature. Channels 1, 2, 4, 5, 7, 8, 10, 11, 13, and 14 record the gas phase temperatures in the reactor. Channels 3, 6, 9, 12, and 15 record the wall temperatures in the reactor with channel 3 recording the wall temperature at the same location as the channel 2 gas phase temperature. Channel 16 is a record of the preheater temperature. Appendix I gives the thermocouple location for each recorder channel.

The thermocouples are "Ceramo" Miniature Chromel - Alumel Thermocouples with a 1/16 inch outside diameter. A "Ceramo" thermocouple consists of the Chromel and Alumel conductors, a ceramic insulation, and a Type 310 Stainless Steel sheath overall. The ceramic insulation protects the conductor wires from each other and from the metal sheath. The hot junction is welded to the tip of the sheath to provide a highly sensitive thermocouple. The thermocouples are mounted in the reactor wall with Swagelok Type 316 fittings which form a pressure seal on the thermocouple sheath. All thermocouple lead wire is asbestos covered Chromel-Alumel lead wire with braided Stainless Steel wire on the outside to act as an electrical shield.

A 1/8 inch Stainless Steel sampling line is connected to the reactor wall below each of the five heaters (Figure 4) to allow sampling at five points. The sample lines pass out through the insulation and connect to 1/8 inch Stainless Steel Hoke Solenoid valves which are activated to sample the reacting stream. Small sample bombs, made from 6 inch lengths



of 3/4 inch Stainless Steel tubing with 1/8 inch Autoclave valves at each end, fasten to the Solenoid valves to receive the gas samples. The sample bombs are stored in an oven at 110°C until analysis is carried out in order to keep all components in the gas phase.

The locations of the sample points are given in Appendix I.

#### D. Temperature Control Circuits

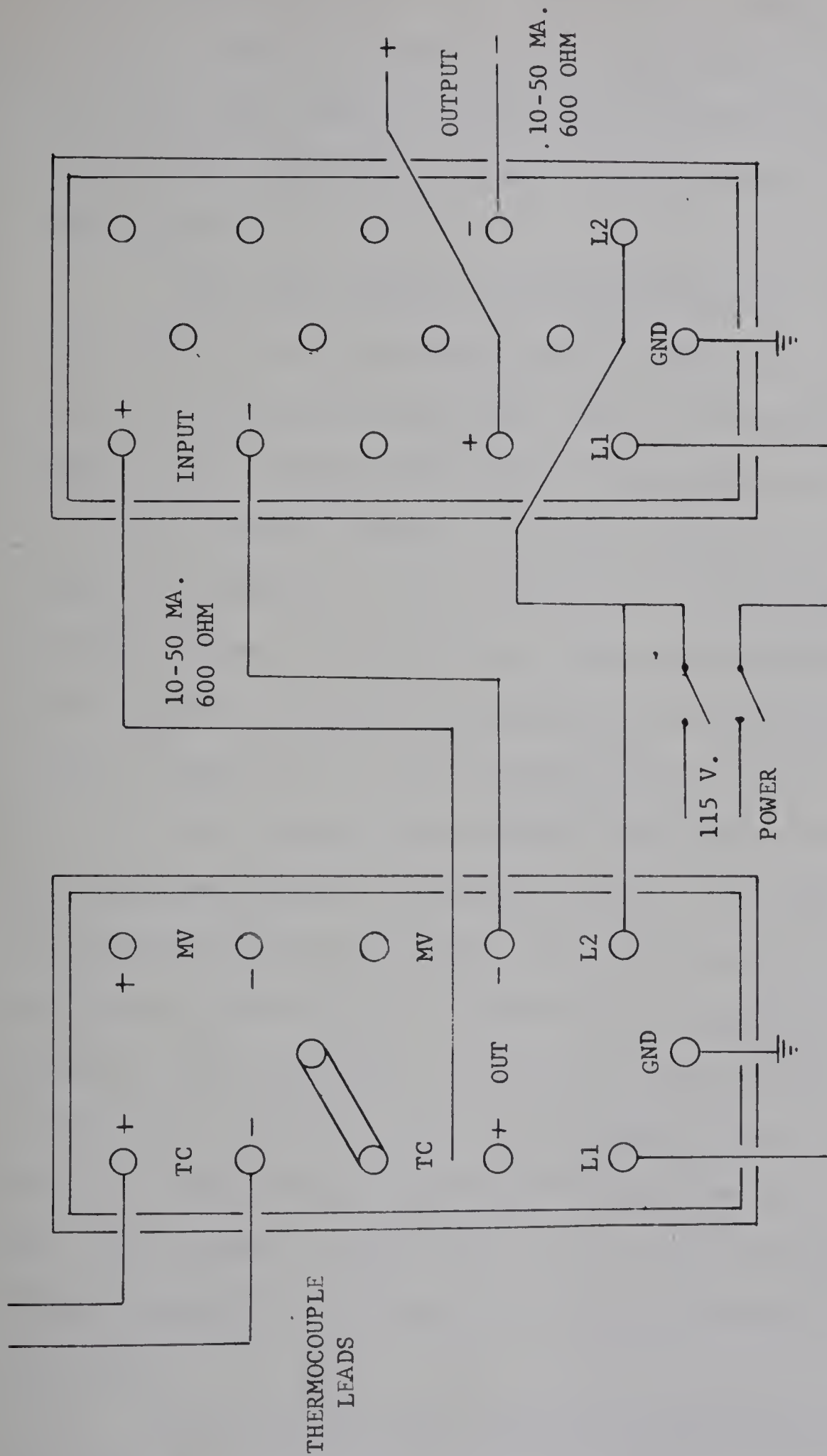
The preheater and reactor temperatures are controlled by the power input to the heaters in each section. The electronic control circuits for the preheater and reactor heaters are identical and are described in detail in Figure 5, 6, and 7.

The electromotive force of the control thermocouple is transmitted to a Foxboro Type 693R EMF to Current Converter which converts the d-c millivolt input signal to a 10 to 50 milliamperes d-c output signal. The range of the converter is set by a Range Unit which controls the "zero" input signal to give a 10 milliamperes output signal, the span of the input signal, and the thermocouple conductor materials. The converter contains a built-in temperature compensator to correct the input signal for ambient temperatures between 20 and 120°F.

The 10 to 50 milliamperes d-c signal from the converter goes to a Foxboro Model 62 Universal Electronic Controller. The controller compares the input signal to the manual set point and produces a 10 to 50 milliamperes d-c output signal







ELECTRONIC  
CONTROLLER

E.M.F. TO CURRENT  
CONVERTER

FIGURE 5: WIRING DIAGRAM - TEMPERATURE CONTROL CIRCUIT



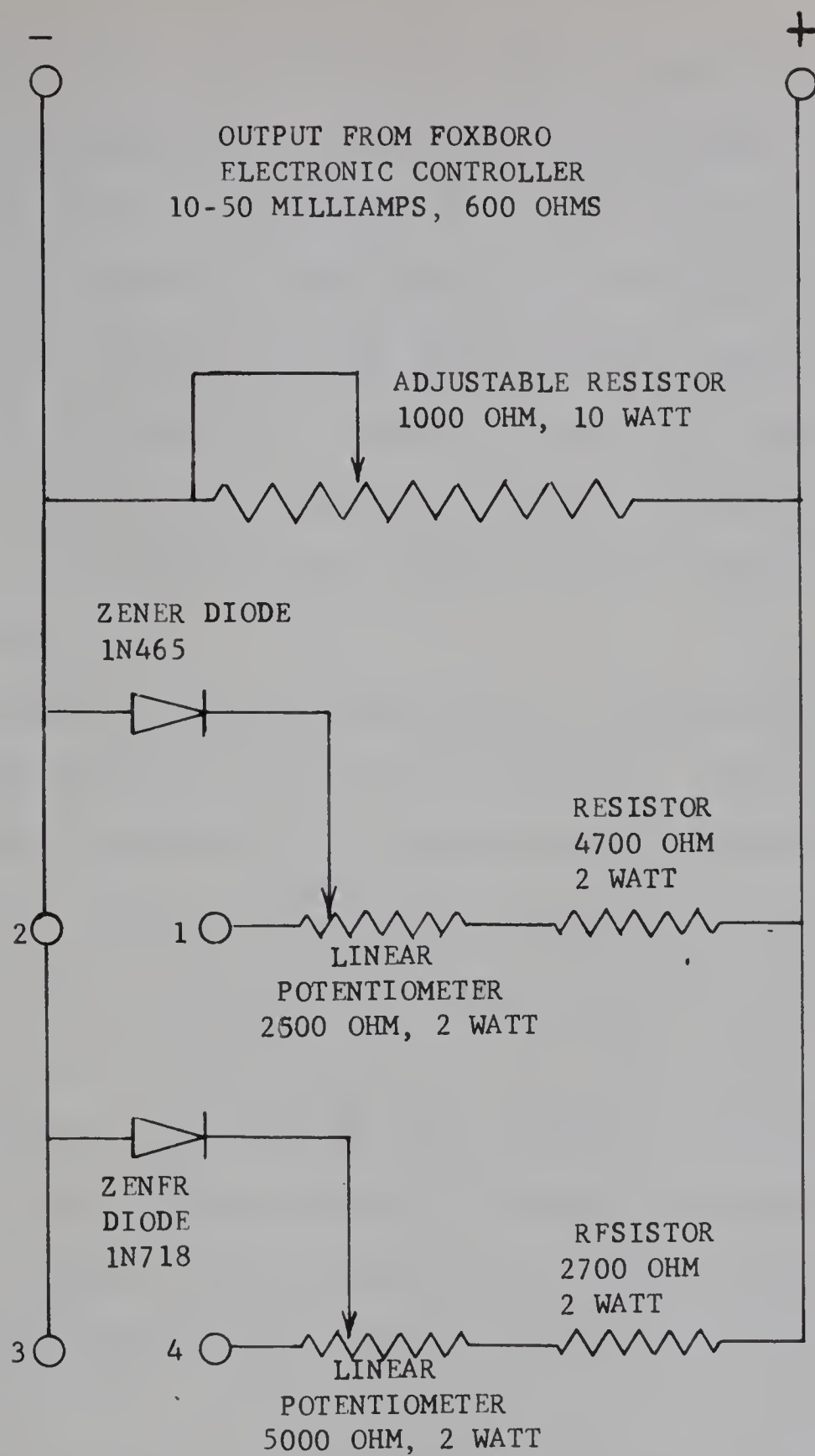
at 600 ohms. The 10 to 50 milliampere output signal acts on the final control element to set the power input to the heaters. The electronic controller operates with a Proportional Band of 20 per cent and a Reset Time of 3.0 minutes for good temperature control.

The final control element is a Vectrol VS6002 Silicontrol Gate Drive which operates gate terminals in two Silicon Controlled Rectifiers Type C50D. The Silicontrol Gate Drive requires a d-c signal of 0 to 3.3 milliamperes. Thus, the 10 to 50 milliampere signal from the controller is adjusted as shown in Figure 6 to give the 0 to 3.3 milliampere signal for the Gate Drive. The 2500 ohm linear potentiometer and Zener Diode 1N465 are used to correct the 10 milliampere controller output signal to a 0 milliampere input signal to the Gate Drive. The 5000 ohm linear potentiometer and Zener Diode 1N718 set the maximum signal to the Gate Drive. In order to protect the heaters against burning out, the maximum signal to the Silicontrol Gate Drive is adjusted at approximately 2.8 milliamperes. The 115 volt a-c line to the Silicontrol Gate Drive must be in the same phase as the single phase 208 volt a-c line to the Silicon Controlled Rectifiers for proper control. For this reason, a 208 volt to 115 volt a-c Hammond Transformer supplies the Gate Drive line voltage from the 208 volt a-c line.

Two Silicon Controlled Rectifiers are required for full wave rectification of the 208 volt, 40 ampere a-c power







1, 2, 3, 4 - GATE DRIVE TERMINALS

FIGURE 6: HEATER CONTROLS - CONTROLLER OUTPUT CIRCUIT



supply to the heaters. A Silicon Controlled Rectifier is a three junction semiconductor device for use in power control requiring the blockage of voltages up to 400 volts and load currents up to 50 amperes. The Controlled Rectifier represents essentially an open circuit with negative anode to cathode voltage if no signal is applied to the gate terminal. However, by applying a gate signal the device rapidly switches to a conducting state and allows current to flow proportional to the gate signal.

The Silicon Controlled Rectifier is connected to the Silicontrol Gate Drive as outlined in Figure 7. The two resistors and Silicon Diodes in each Rectifier circuit are for protection of the Gate Drive and controller. Silicon Controlled Rectifiers occasionally fail by losing their ability to block forward voltage and becoming a dead short. The primary short path is frequently from anode to gate which means that the anode voltage appears between the gate and the cathode for an instant before punching through to the cathode. This voltage could destroy the control system if it was unprotected.

A 0 to 50 ampere a-c ammeter in the power line from the Silicon Controlled Rectifiers to the heaters measures the current flowing through the heaters.





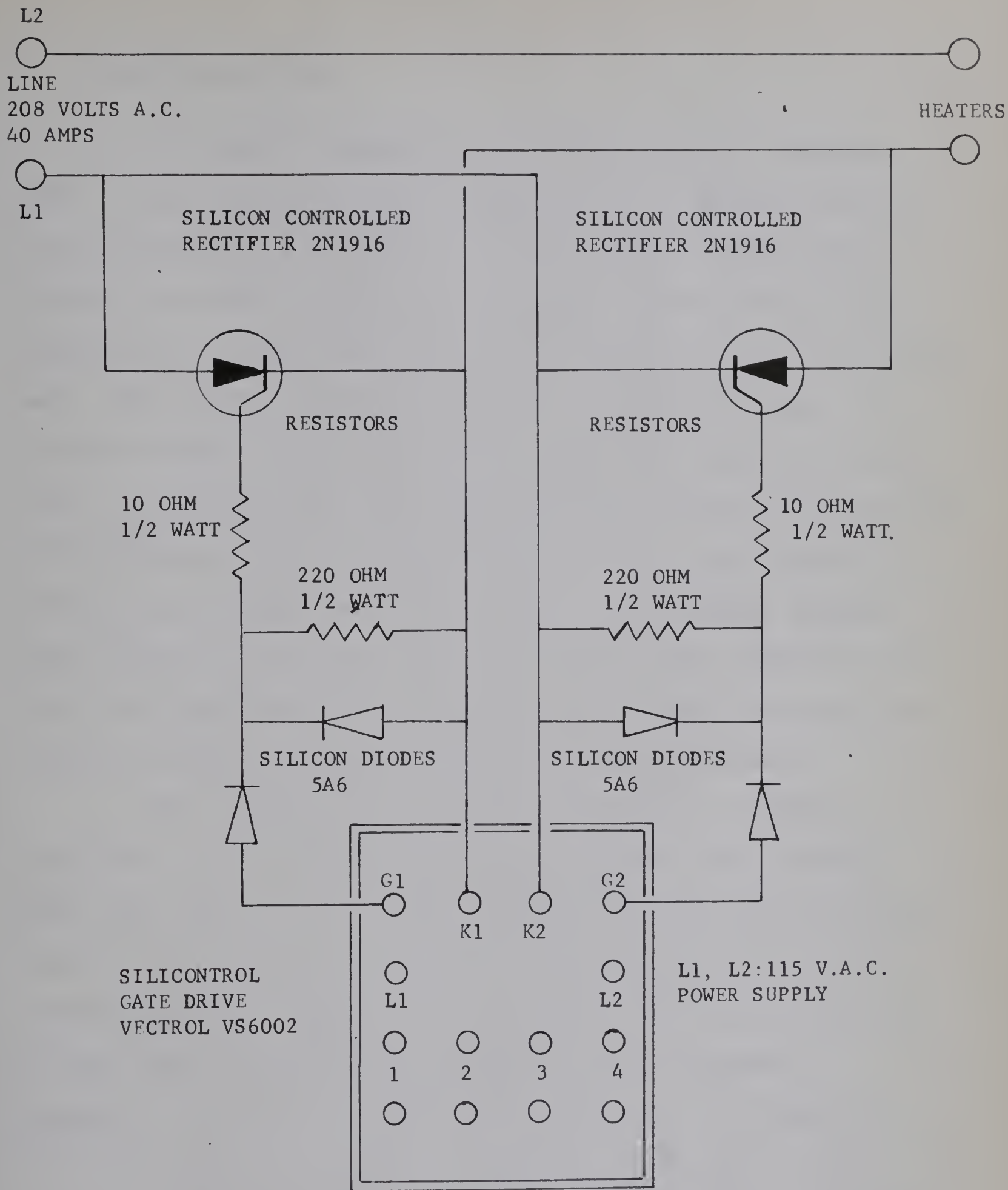


FIGURE 7: HEATER CONTROLS - GATE DRIVE CIRCUIT



#### E. Product Analysis

All product samples were analysed using a Burrell Model KD Gas Chromatograph equipped with a Thermal Conductivity detector. A Sargent millivolt recorder Model SR recorded the output of the chromatograph. Helium at an inlet pressure of 40 psig was used as the carrier gas for all analyses. The helium, before entering the chromatographic unit, passed through a drier cartridge supplied by Burrell Corporation. The helium flow rate was regulated for both the carrier and reference sides by Nupro Metering Valves and checked by timing soap bubbles in a gas burette. All product samples were injected into the columns through the gas sampler built into the Chromatograph. The sample size could be changed by switching sampler tubes of 1/8 inch Stainless Steel.

Four columns were required to effect a complete separation of the components in the samples. All columns were made from 1/4 inch copper tubing with 3/16 inch Swagelok fittings on each end and wound into spirals to fit into the temperature bath cabinet. The columns, their operating conditions, and the components separated are as follows:

Column 1: A 25 foot long column packed with 30 weight per cent Ucon LB1800-X Lubricant made by the Union Carbide Chemicals Company on 30 to 60 mesh Celite.  
Components Separated: Hydrocarbon groups according to the number of carbon atoms up to and





including C<sub>4</sub> hydrocarbons, higher molecular weight hydrocarbons and all oxygenated products.

Column Temperature: 80°C for the first 7 minutes followed by a 10°C/minute temperature rise to 150°C.

Carrier Flow Rate: 45 mls/minute

Reference Flow Rate: 30 mls/minute

Detector Current: 200 milliamperes

Gas Sampler: 8.0 inch long; 0.49 c.c. volume.

Column 2: A 25 foot long column packed with 3 weight per cent Di-n-decyl Phthalate made by Eastman Organic Chemicals on Medium Activity Silica Gel, 30 to 60 mesh, supplied by Burrell Corporation.

Components Separated: C<sub>2</sub> to C<sub>4</sub> hydrocarbons and olefins and carbon dioxide.

Column Temperature: 100°C for the first 8 minutes followed by a 15°C/minute temperature rise to 150°C.

Carrier Flow Rate: 24 mls/minute

Reference Flow Rate: 30 mls/minute

Detector Current: 200 milliamperes

Gas Sampler: 5.5 inches long; 0.28 c.c. volume.

Column 3: A 16 foot long column packed with Type 13X Molecular Sieves, 30 to 60 mesh, supplied by Burrell Corporation.

Components Separated: Ethane and ethylene

Column Temperature: 175°C



Carrier Flow Rate: 50 mls/minute

Reference Flow Rate: 30 mls/minute

Detector Current: 200 milliamperes

Gas Sampler: 5.5 inches long; 0.28 c.c. volume.

Column 4: A 16 foot long column packed with High Activity Charcoal, 40 to 60 mesh, supplied by Burrell Corporation for the first 8 feet followed by Molecular Sieves Type 13X.

Components Separated: Hydrogen, oxygen, nitrogen, carbon monoxide, methane.

Column Temperature: 80°F

Carrier Flow Rate: 60 mls/minute

Reference Flow Rate: 30 mls/minute

Detector Current: 250 milliamperes

Gas Sampler: 5.5 inches long; 0.28 c.c. volume.

The components were identified by their retention times. The retention time of a component is the time taken from sample injection until the maximum point of the peak appears on the chromatogram. Retention times for the various components and examples of chromatograms for each chromatographic column are reported in Appendix II.

#### F. Operating Procedure

The general operating procedure required to make any run was as follows:





1. The main air supply was turned on and all water traps and filters were blown out. The process air pressure was set at a value of 20 psig above the reactor pressure. The instrument air pressure was set at 20 psig. The bypass valve between the process air line and the n-butane feed line was opened and air was passed through the preheater coils and reactor. The steam ejector system was turned on.

2. The electrical heaters in the preheater and reactor were turned on.

3. The n-butane feed tanks were filled from storage and pressurized with nitrogen to a pressure 20 psig above the reactor pressure.

4. Ice was placed in the recorder thermocouple cold junction bath. The temperature recorder was calibrated using a d-c millivolt input from a Leeds and Northrup 8686 Potentiometer to the recorder channel 15.

5. Sample bombs were evacuated and connected to the sample lines.

6. When the reactor and preheater had approached reaction temperature, the bypass valve to the n-butane feed line was closed. n-Butane and air feeds were started and the desired flow rates set on the pneumatic controllers. The reactor pressure was set on the pressure controller. The preheater and reactor temperature controllers were set at the reaction temperature desired. The temperature recorder was turned on. The recorder charts in the n-butane and air flow



controllers were turned on.

7. When steady state conditions were attained as indicated by the temperature profiles the inlet valves to the sample bombs were opened and the solenoid valves actuated. The sample bombs were flushed out twice with gas samples and the third sample was retained for analysis.

8. The electrical heaters, the n-butane feed, the temperature recorder, and the flow recorders were all turned off. The bypass valve to the n-butane feed line was opened to allow air to pass through the system while cooling. The sample bombs were removed and stored in an oven at  $110^{\circ}\text{C}$ . The steam ejector system was turned off.

9. When the preheater and reactor returned to room temperature, the main air supply was turned off.

10. Analysis was carried out on the samples by installing the proper column, setting the helium flow rates on the carrier and reference sides, and setting the column temperature. When the chromatograph reached equilibrium conditions, a sample was injected into the column through the gas sampler. The chromatogram was traced on to the Sargent recorder chart. The temperature programmer was turned on at the given time for the columns that required temperature programming. After each sample analysis was completed, the column temperature was returned to its initial temperature, if the temperature programmer had been used, before the next sample was injected.





## G. Calibration of Equipment

Calibration of the Integral Orifice D/P Cells for the n-butane and air feed streams, the Pressure Transmitter, and the thermocouples was carried out prior to the start of the experimental program. Calibration procedures and curves are presented in Appendix III.



## EXPERIMENTAL PROGRAM

### A. Reaction Variables

Preliminary experimentation indicated that significant reaction took place between the n-butane and oxygen at an inlet temperature of 700°F, a pressure of 40 psig and inlet oxygen concentrations of 6 to 10 mole per cent. These experiments gave an optimum residence time of 1.2 to 1.4 seconds based on the inlet conditions. Such a residence time permitted sampling at the beginning of the reaction, during the period of high reaction rate, and in the period when little reaction took place. Gas phase temperature profiles clearly indicated each region of the reaction.

Based on the preliminary investigation, it was decided to carry out experiments at different inlet temperatures and oxygen concentrations with a constant pressure of 53.5 psia (40 psig) and an overall residence time between 1.2 and 1.3 seconds. The three inlet temperatures investigated were 685, 705, and 725°F although individual run inlet temperatures varied slightly. Inlet oxygen concentrations of 6.45, 7.25, and 8.10 mole per cent were studied at each temperature. Once again, the inlet oxygen concentration for any individual run varied a slight amount from the desired value. In all of the experimental runs the oxygen was obtained from air which resulted in a definite percentage of nitrogen in all reaction gases.





Three runs were made with n-butane only to determine the effect of the cracking reactions at the temperatures used in the oxidation experiments. The experiments were made at temperatures of 700, 792, and 909<sup>o</sup>F with a reactor pressure of 53.5 psia and an average residence time of 1.31 seconds calculated at the fourth sample point rather than the reactor exit. This procedure was used as it was impossible to obtain a high enough flow rate of n-butane, without changing orifice plates in the D/P Cell and recalibrating it, to give the required residence time at the reactor exit. Details of each experimental run are given in Table 1.

#### B. Raw Materials

The butane used in the preliminary runs was supplied by Canadian Natural Gas Liquids Limited and contained a ratio of n-butane to i-butane of approximately 2 to 1 and traces of propane and pentanes. This butane was satisfactory for the preliminary runs as they served only to define the field of study and to provide operating experience.

All runs in the experimental program were made with C.P. Grade n-butane supplied by Matheson of Canada Limited. Chromatographic analysis of samples of the n-butane gave a composition of 99.6 mole per cent n-butane and 0.4 mole per cent i-butane which was well within the specified composition. The absence of any other hydrocarbons or olefins was confirmed by the analysis. No attempt was made to correct the



Table 1

Experimental Run Details

Run Number	Inlet Temperature °F	Pressure psia	Reactor Inlet Concentrations		Inlet Concentrations		Residence Time* Seconds	Inlet Reynolds Number
			Oxygen	Mole Percent Nitrogen	n-Butane			
10	732	53.5	8.48	31.89	59.63	1.52	4578	
11	705	53.5	6.35	23.90	69.75	1.38	6000	
12	704	53.5	6.29	23.68	70.03	1.16	7129	
13	705	53.5	6.47	24.33	69.20	1.29	6369	
14	696	53.5	6.47	24.33	69.20	1.30	6413	
15	727	53.5	6.45	24.25	69.30	1.26	6294	
16	702	53.5	7.25	27.27	65.48	1.22	6467	1
17	681	53.5	7.24	27.23	65.53	1.23	6636	59
18	723	53.5	7.25	27.29	65.46	1.22	6240	1
19	685	57.5	8.09	30.41	61.50	1.32	6237	
20	702	53.5	8.09	30.41	61.50	1.21	6158	
21	687	53.5	8.10	30.47	61.43	1.21	6295	
22	723	53.5	8.06	30.34	61.60	1.20	6004	
26	699	53.5	8.12	30.54	61.34	1.22	6156	
23	700	53.5			100.0	1.30		
24	792	53.5			100.0	1.33		
25	909	53.5			100.0	1.32		

\* Residence times corrected for reaction conditions are described in Appendix IX.





product analysis for the presence of i-butane. It was reported as a component in the product sample.

All air for the experimental runs was obtained from a compressed air line and, after the removal of traces of moisture and oil, was fed directly to the reactor. Chromatographic analysis of several samples of the air taken at intervals during the experimental program showed the presence of no trace components.

### C. Chromatograph Analysis

All components were identified by their retention times in the chromatograph column. The retention time for each expected compound was determined by running a pure sample of the compound through the column under the same conditions used for the product analysis. Retention times of the gaseous components were checked by analysing known mixtures of the gases which had compositions similar to the gaseous components in the reacting system. This procedure was necessary to check the effect of individual compounds on each other and to verify that no components had switched order.

In order to confirm the identity of many oxygenated products a special liquid sample was collected at the reactor exit during one of the runs. The liquid sample was collected by allowing a portion of the product gas stream to pass through a receiver in an ice-water bath. The receiver retained the components that condensed and allowed the gas to



escape to the atmosphere. A small portion of the liquid sample was then analysed on the Ucon column and the retention time and peak area were recorded for each component. Verification of the identity of the components was carried out by adding a very small amount of a known compound to a part of the liquid, running the sample through the chromatograph, and determining which component peak area increased relative to all others.

The retention time for each component is given in Appendix II for all columns. The same retention time is given for more than one component on a specific column if these components were not separated and appeared as one peak.

The peak area for each component was measured by one of two methods. If the component peak was sharp the peak area was determined by assuming that the area was triangular and multiplying the peak height by the width at half the height. All other peak areas were measured with an Ott Compensating Planimeter supplied by Burrell Corporation for use with gas chromatographs.

The peak area for each component was converted to a mole fraction by using a relative response factor as described by Rosie and Grob(34) and Messner and co-workers(25). They investigated the relative molar responses of a number of hydrocarbons and oxygenated compounds over a wide range of column temperatures, concentrations, and carrier gas flow rates. A correlation was found to exist between the relative





thermal detector response and molecular weight within a structurally similar homologous series. The correlation was independent of the column conditions as long as helium was the carrier gas, the detectors were thermal detectors, and the temperature was constant. All responses were related to benzene at 100.

As Messner and co-workers(25) did not give relative response factors for aldehydes, several known mixtures of acetaldehyde, propionaldehyde, and butyraldehyde in benzene were analysed. The relative response factor for formaldehyde was calculated by extrapolating the response factors obtained for the other aldehydes.

The relative response factors were applicable as long as a constant temperature was maintained in the chromatograph column. Because temperature programming was used to give better component separations, correction factors were calculated to correct for the temperature variations. The correction factors were determined by running pure samples of the components through the chromatograph columns at the base temperature and with the temperature programmer in operation and comparing peak areas. Peak areas were found to increase when the temperature programmer was used.

The relative response factors and correction factors are given in Appendix II.



## DISCUSSION OF RESULTS

### A. Equipment

The equipment can be described best in two sections consisting of the control accuracy and flow conditions in the reactor.

The control of n-butane and air flow rates, reactor pressure, and reaction temperature was very good because of the pneumatic and electronic controllers. The inlet n-butane and air flow rates produced a maximum deviation of  $\pm 0.5$  per cent of the full recorder chart range from the desired set point. The  $\pm 0.5$  per cent deviation on the recorder chart gave a maximum error in the weight rate of flow of the n-butane and air of  $\pm 1$  per cent of the desired flow.

The reactor pressure was recorded on the same chart as the n-butane flow rate and varied from the set point by only  $\pm 0.2$  per cent of the full chart scale. The major portion of the error in the pressure was due to errors in reading the chart accurately. Calibration of the pressure transmitter indicated that the chart recorded the gauge pressure accurately. However, the accuracy with which the chart could be read was almost  $\pm 0.2$  per cent of the scale. The error introduced in the pressure reading was  $\pm 0.4$  psi, which at a reactor pressure of 40 psig, was  $\pm 1$  per cent of the set pressure. During each experimental run the atmospheric pressure was determined and the transmitter pressure was then corrected to give an absolute







pressure of 53.5 psia. The pressure in run 19 was at 57.5 psia due to a high pressure drop across the ceramic filter in the exit line. The high pressure drop was caused because the filter was partially plugged with carbon particles. The filter was cleaned and reinstalled prior to experimental run 20.

The temperature controller for the preheater maintained the millivolt recording of the thermocouple in the preheater within  $\pm 0.04$  millivolts of the desired reading. This corresponded to a variation from the set temperature of  $\pm 2^{\circ}\text{F}$  according to the temperature recorder. All the thermocouples were calibrated, as described in Appendix III, and found to be within  $\pm 3^{\circ}\text{F}$  of the correct temperature. The maximum error due to temperature fluctuations and thermocouple inaccuracy, in the preheater control temperature was  $\pm 5^{\circ}\text{F}$ . All thermocouples in the gas phase indicated a temperature below the actual temperature because of the heat transferred from the thermocouples by conduction and radiation to the reactor wall. This error will be discussed later in the section on reactor temperature profiles.

The temperature controller for the reactor was used only for heating the reactor to reaction temperature in most cases due to poor positioning of the control thermocouple. For most of the experimental runs, the control thermocouple was in the reaction zone and measured a temperature higher than the control temperature. For the experiments with n-butane only, runs 23, 24, and 25, the controller maintained



the temperature at the control point within the same accuracy as the preheater temperature controller.

The flow conditions in the reactor are described by the Reynolds number which indicates whether or not turbulent flow exists and by the Peclet number which is a measure of axial dispersion or back mixing in the reactor.

The flow into the reactor was turbulent as indicated by the Reynolds number calculated for each run at the entrance conditions and reported in Table 1. According to McCabe and Smith (23), flow is turbulent at Reynolds numbers above 4000 under ordinary flow conditions. The average Reynolds number, at the entrance, was 6500 which is well into the turbulent range.

The Reynolds number, being a function of the tube diameter, the mass flow rate per unit area, and the viscosity of the gas stream, depends only on the viscosity for any run at any position in the reactor. The viscosity of gases increases with temperature, in general, but in the reacting system components of lower molecular weight are formed with lower viscosity. As a result, it was impossible to calculate the effect of temperature and reaction on the viscosity and the Reynolds number. Because the temperature and reaction have opposing effects on the viscosity of the gas, it was assumed that the viscosity did not change sufficiently throughout the reactor to alter the Reynolds number and flow pattern.

The Peclet number for mass transfer is a measure of





axial dispersion in the reactor. Since the transport of heat and mass are by the same mechanism, it is reasonable to suppose that, for turbulent diffusion and heat transfer, the Peclet numbers for heat and mass transfer are identical. Consequently, the Peclet number for heat transfer was determined from the fluid and flow properties of the system and equated to the Peclet number for mass transfer. The Peclet number for heat transfer is the Reynolds number multiplied by the Prandtl number and has an average value of 10,000 at the reactor entrance. According to Kramers and Westerterp(19), an ideal tubular reactor, with plug flow, has a value of the inverse of the Peclet number equal to zero and a reactor with a small amount of dispersion has a value of the inverse of the Peclet number equal to 0.002. For the reactor used in the experimental runs, the Peclet number at the entrance was 10,000 and the inverse was 0.0001. This value, when it was compared to the values given by Kramers and Westerterp, verified the assumption of plug flow in the reactor.

#### B. Product Analysis

The analysis of the product samples and the use of the relative response factors to calculate the mole per cent of each component was quite accurate as indicated by the analysis of test samples and the carbon, hydrogen, and oxygen balances for each sample. Carbon, hydrogen, and oxygen balances are given in Appendix VII.



In order to check the accuracy of the use of the relative response factors as described by Messner and co-workers(25), a test sample of known composition was prepared and analysed on the gas chromatograph. The composition was then calculated and compared to the true composition. Results of the test sample analysis are given in Table 2. Table 3 presents the results of analysis made on a test sample by Rosie and Grob(34). Use of the relative response factors gave a calculated mole per cent within  $\pm 2.5$  per cent of the true value as compared to an error or  $\pm 8$  per cent if the area per cent is assumed to be equal to the weight per cent of each component.

The accuracy of the analysis of the product samples is determined, as well, by the carbon, hydrogen, and oxygen balances.\* The carbon balances for all the experimental samples were between 97 and 103 per cent with the majority of them between 98 and 100 per cent. The hydrogen balances were between 92 and 100 per cent for all samples with the average between 95 and 98 per cent. The oxygen balance was the poorest, varying from 80 to 100 per cent. The carbon and hydrogen balances were good and served as a check on the use of the relative response factors for the components.

There were two reasons for the low oxygen balance. The chromatographic analysis for both carbon dioxide and water were doubtful in many cases due to poor separation on the column.

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\* Carbon and hydrogen balances based on the n-butane reacted are given in Appendix VIII.





Table 2

Test Samples with Compositions Calculated

Using Relative Responses

Compound	True Wt. %	True Mole %	Observed Area %	Calculated Mole %
Propionaldehyde	27.1	28.1	25.8	27.8
Methanol	1.8	3.4	2.1	3.2
Ethanol	17.6	23.1	18.5	22.7
Methyl Ethyl Ketone	17.7	14.9	18.2	15.1
n-Propanol	17.9	18.0	18.5	18.2
Diethyl Ketone	17.9	12.5	16.9	13.0

Table 3

Relative Response Analysis of Sample

by Rosie and Grob(34)

Compound	True Wt. %	True Mole %	Observed Area %	Calculated Mole %
n-Pentane	5.56	7.52	6.48	7.75
2,3-Dimethyl Butane	7.72	8.75	8.12	8.80
2,2-Dimethyl Pentane	8.17	7.96	8.45	7.98
2-Methyl Hexane	6.15	5.99	6.36	5.87
n-Heptane	7.40	7.21	8.00	7.03
Benzene	14.80	18.50	15.23	19.14
1,4-Dimethyl Cyclohexane	11.11	9.66	11.21	9.65
Ethyl benzene	11.46	10.53	10.48	10.21
o-Xylene	13.42	12.35	13.19	12.76
n-Propylbenzene	14.21	11.53	12.48	10.81



The carbon dioxide was not separated on any column as none could be found to give a distinct separation of ethylene and carbon dioxide. Consequently, it was determined by a difference of areas in two different columns. The Silica Gel column, previously referred to as the column with 3 per cent di-n-decylphthalate on Silica Gel in the section on equipment detail, did not separate ethylene and carbon dioxide. The carbon dioxide caused tailing of the peak which made accurate area determination difficult. The ethylene composition was determined, relative to ethane, from the Molecular Sieve column and carbon dioxide was calculated by the difference between the area of the ethylene peak and the area of the ethylene and carbon dioxide peak. For these reasons, the carbon dioxide analysis was poor.

The water analysis was inaccurate mainly because of poor separation on the Ucon column. The water peak was not symmetrical, as can be seen in Figure II-1, and tailed badly. At higher water concentrations the water peak frequently overlapped the methanol peak and samples had to be re-run for more accurate analysis.

The questionable water and carbon dioxide analyses caused the low oxygen balance as much of the oxygen, after reacting, is contained in either the water or the carbon dioxide. Another cause of the low oxygen balance was due to the fact that the per cent oxygen in the feed stream was always low, between 6 and 8 per cent and, any error in analysis





had a much larger effect on the oxygen balance than on either the carbon or hydrogen balances.

### C. Temperature Profiles in the Reactor

Temperature profiles were measured in the reacting gas stream by ten thermocouples. All temperatures are given in Table IV-1 for all of the experimental runs. The temperature profiles for several runs are described in Figure 8 which shows the effect of inlet temperature and Figure 16 which depicts the effect of oxygen concentration. These figures will be discussed further in the sections referring to the effect of reaction variables on the overall reaction.

Errors in reading the temperature recording and inaccuracies in the thermocouple millivolt readings were only  $\pm 5^{\circ}\text{F}$  as previously outlined for the control thermocouples. However, there was a further error in the gas phase thermocouples which was caused by radiant and conductive heat transfer from the thermocouple sheath to the reactor wall. The magnitude of this error is calculated in Appendix V and is in the order of  $12^{\circ}\text{F}$  when there is a difference of  $80^{\circ}\text{F}$  between the reactor wall temperature and the temperature of the thermocouple tip at a wall temperature of  $820^{\circ}\text{F}$ . The thermocouple reads a temperature below the true gas temperature by  $12^{\circ}\text{F}$  which gives an actual gas temperature of  $912^{\circ}\text{F}$ . The conditions chosen in the calculation of the thermocouple correction were average with respect to temperature and flow rates. The



difference between the wall temperature and the temperature of the thermocouple tip of  $80^{\circ}\text{F}$  was a maximum value, except for the difference at the reactor exit, and in most cases was approximately  $60^{\circ}\text{F}$ . At the reactor exit, the wall temperature was approximately  $230^{\circ}\text{F}$  below the gas phase thermocouple reading due to the location of the thermocouples. The thermocouples were positioned at a point just above the reactor exit flange and, at that point, the reactor wall was uninsulated. This caused a rapid decrease in wall temperature due to heat losses to the surroundings.

No attempt was made to correct any of the gas phase temperature because of the difficulty involved in determining heat transfer coefficients between the reacting gas stream and the thermocouple sheath. Flow conditions were known at the reactor entrance but were not known accurately throughout the reactor as it was impossible to determine the effect of the reaction and the increase in temperature on the properties of the gas stream. Thus, the heat transfer coefficient was determined from an empirical equation for the entrance conditions only and assumed to be unchanged. Since individual thermocouple corrections could be calculated using only the entrance heat transfer coefficient and would, therefore, become an average correction, it was decided to report the magnitude of the error only.

The three experimental runs with n-butane only, runs 23, 24, and 25, did not have the same errors in thermo-





couple readings because the difference between the wall and indicated temperature was  $14^{\circ}\text{F}$  at a maximum and at an average of  $8^{\circ}\text{F}$ . The wall temperature was always higher than the gas temperature as heat was being transferred from the wall to the gas stream. Errors due to radiation and conduction to the thermocouples caused only 1 or  $2^{\circ}\text{F}$  errors in the readings.

For any experimental run for the reaction between n-butane and oxygen, the indicated gas temperature decreased gradually during the induction period and then increased rapidly with the start of the period of rapid reaction. After the period of rapid reaction, the temperature again decreased.

The gradual decrease in temperature in the induction period was due to the transfer of heat from the gas phase to the reactor wall. The control thermocouple for the reactor temperature control circuit was positioned so that it was in the reaction zone for the majority of the experimental runs and was at a temperature too high for control. As a result, the reactor wall at the entrance was cooler than the gas stream and heat was transferred from the gas to the reactor wall.

During the period of rapid reaction, the gas temperature increased rapidly to a peak temperature approximately  $400^{\circ}\text{F}$  above the inlet temperature within about 0.2 seconds. During this period most of the reaction took place and the high exothermic heat of reaction caused the rapid increase in temperature. Any thermocouples located in this section of



the reactor, between the initial temperature and the peak temperature gave readings that fluctuated as much as  $20^{\circ}\text{F}$  due to slight fluctuations in air or n-butane flow rates at the entrance.

After the rapid reaction period, most of the oxygen was consumed and very little reaction took place. In this phase of the reaction system, heat was transferred from the gas stream to the reactor wall which caused the decrease in gas phase temperatures.

The reactor wall temperature was, in most cases, between  $60$  and  $80^{\circ}\text{F}$  lower than the indicated gas temperature in the reaction zone because of the high rate of heat transfer from the gas stream to the wall. With the electrical heaters and insulation around the reactor wall this heat could not be transferred to the surroundings at a rate sufficient to keep the wall temperature more uniform. The electrical heaters were not on but acted as insulation.

Even when the reactor electrical heaters were on during the run, as was the case for the three runs with n-butane only, the reactor wall temperature and, as a result, the gas temperatures were not constant. The temperature profiles given in Table IV-1 for runs 23, 24, and 25 show that the temperature dropped gradually at the reactor entrance and returned to the control temperature at thermocouple number 6 which was at the same location as the reactor control thermocouple. Beyond this point, the temperature increased gradually





to a value about 40°F above the control temperature at the reactor exit. Thus, the electrical heaters did not provide a constant wall temperature even for the experimental runs in which no reaction took place.

#### D. Products Formed in the Reaction

At temperatures of 685, 705, and 725°F, reaction occurred between the oxygen and the n-butane to give a large number of products. The methods used in calculating the experimental results are outlined in Appendix VI and all the results are given in Appendix VII.

The results indicated that the predominant reactions were the reactions leading to olefins and lower molecular weight hydrocarbons. For the experimental runs, approximately 60 per cent of the reacted n-butane formed olefins, 10 per cent formed methane and ethane, 10 per cent formed carbon oxides, and the remaining 20 per cent formed oxygenated products. A more detailed description of the components formed is given in the sections on the effect of reaction variables on the reaction.

The three runs that were carried out to determine the extent of the cracking reactions confirmed that the cracking reactions were not important at the temperatures used for the reactor inlet. No reaction occurred for the runs at 700 and 792°F as no products were identified in the chromatographic analysis except the small percentage of i-butane present



in the feed stream and the n-butane. At  $909^{\circ}\text{F}$  very little reaction occurred and ethylene and propylene were identified in the product sample only in trace quantities. At the temperatures obtained during the period of rapid reaction cracking reactions may have been significant but the extent of these reactions could not be determined because the temperature control circuits were designed to give a maximum temperature of approximately  $900^{\circ}\text{F}$ .

The reproducibility of the experimental conditions was checked by making two identical runs. Run number 20 and 26 are similar except for a  $3^{\circ}\text{F}$  difference in reactor entrance temperature. The temperature profiles, the product distribution, and the overall conversion of both n-butane and oxygen were in good agreement. Analysis of three samples only for run 20 was caused by leaks in two sample bombs and the subsequent loss of the product samples.

#### E. Effect of Temperature on the Reaction

The inlet temperature had a very significant effect on the induction period as shown in Figure 8. The experimental runs used in the plots are runs 16, 17, and 18 at respective inlet temperatures of 702, 681, and  $723^{\circ}\text{F}$ . For an inlet temperature of  $681^{\circ}\text{F}$ , the induction period was approximately 0.5 seconds but it decreased to 0.3 seconds for an inlet temperature of  $702^{\circ}\text{F}$  and to 0.2 seconds for an inlet temperature of  $723^{\circ}\text{F}$ . This effect of temperature on the





- 702°F
- × 681°F
- 723°F

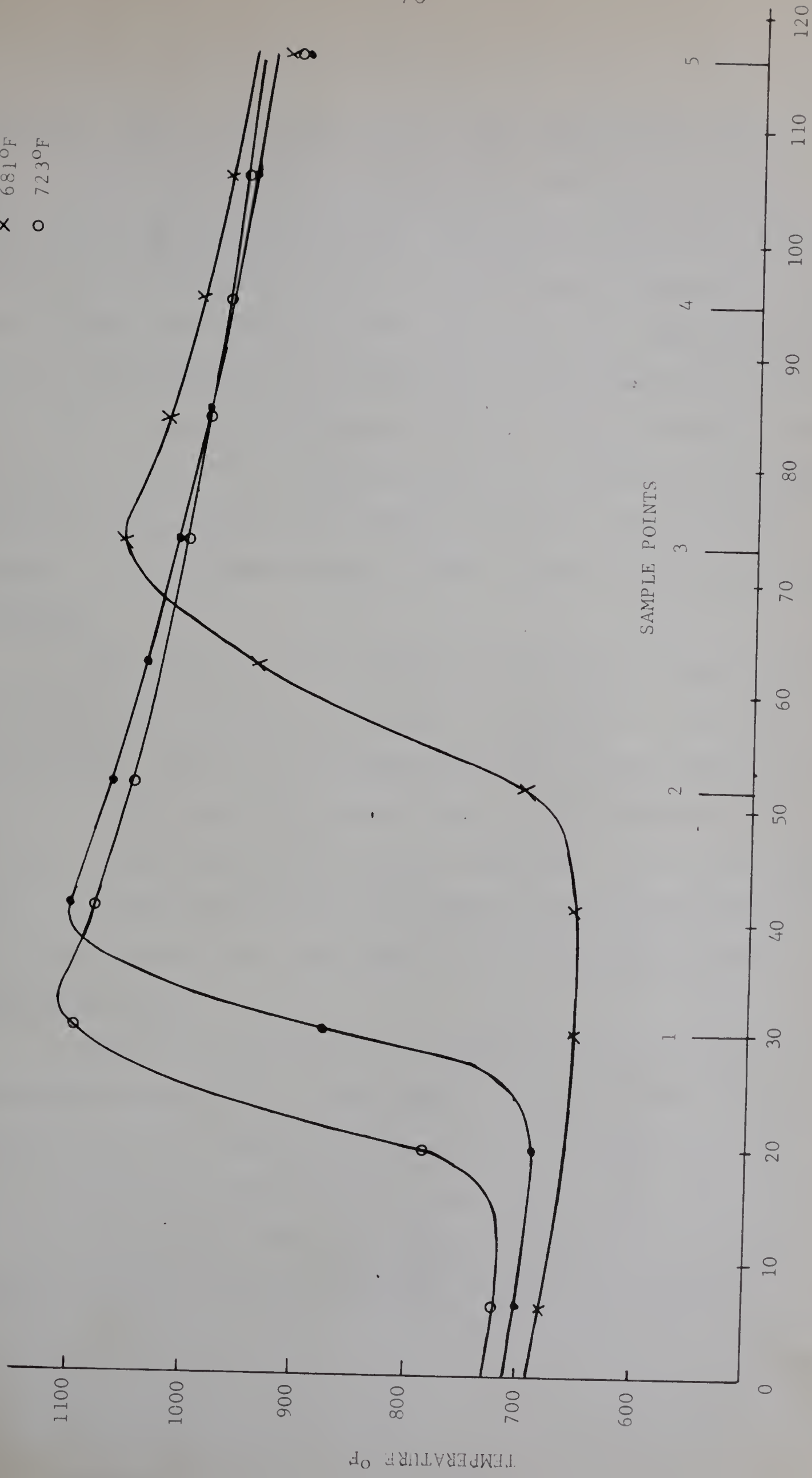


FIGURE 8: REACTION TEMPERATURE PROFILES - EFFECT OF INLET TEMPERATURE



induction period was noted for all the experimental runs.

The length of time during which the rapid reaction took place was dependent on the inlet temperature to a certain extent but, not nearly as much as the induction period. At inlet temperatures around 685°F, the period of rapid reaction lasted approximately 0.2 seconds but at temperatures of 705 and 725°F it was approximately 0.15 seconds in duration. All residence times in the reactor were given based on the inlet conditions even though the actual residence time was less because of increased velocity in the reactor as the reaction proceeded.

The oxygen in the reaction system was consumed rapidly following the induction period up to a value of 95 per cent conversion. Figure 9 indicates that part of the oxygen was used up in the induction period but that the majority of it reacted during the period of rapid reaction. The 95 per cent limit in oxygen conversion was common to all experiments and was caused by the low concentration of the oxygen in the reacting stream.

Very little conversion of the n-butane occurred during the induction period, as outlined in Figure 9, but it increased rapidly once the reaction started up to a maximum value of 20 to 30 per cent conversion at the reactor exit. For most of the experimental runs, the overall conversion of the n-butane increased with an increase in inlet temperature.





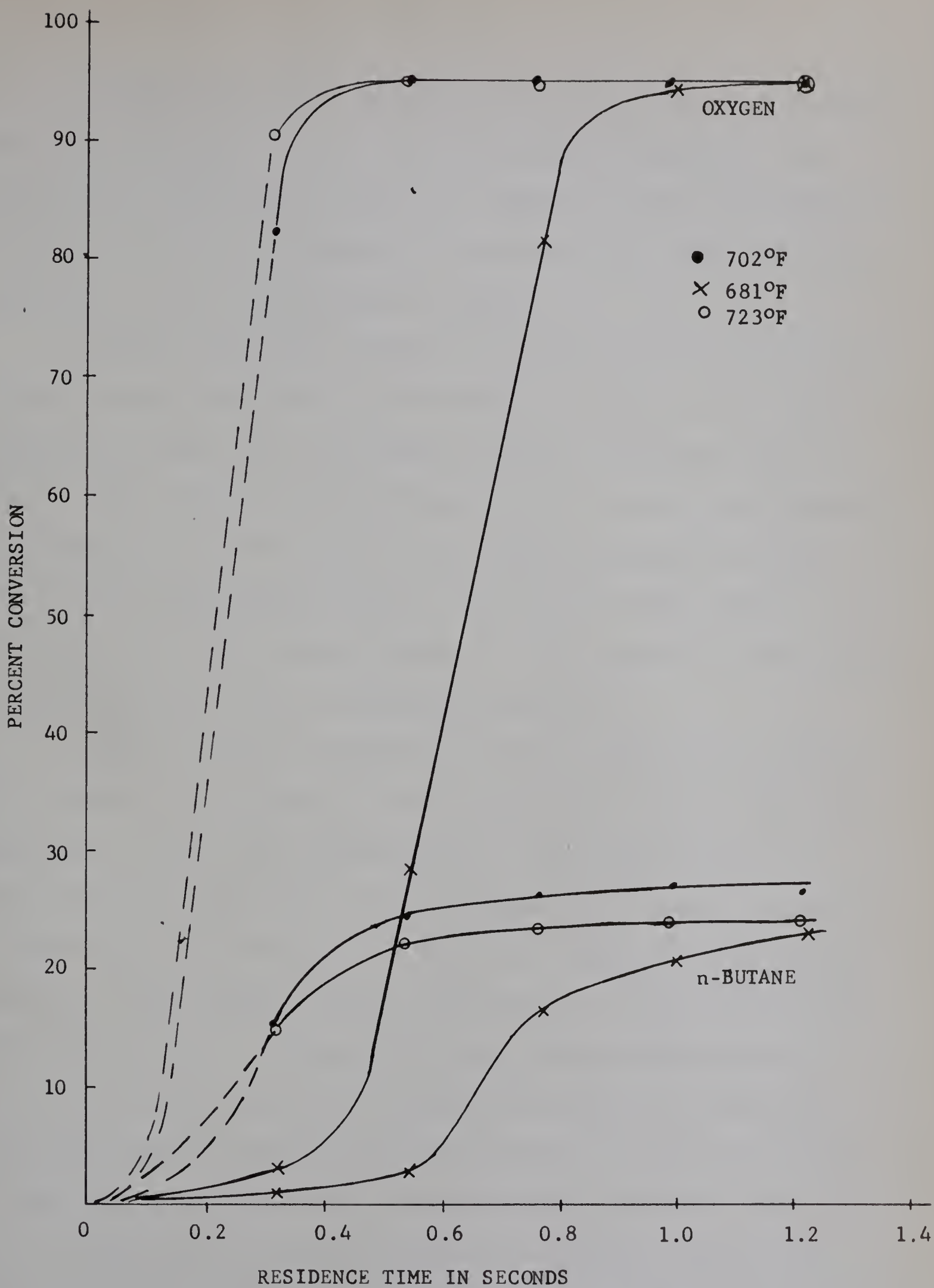


FIGURE 9: EFFECT OF TEMPERATURE ON CONVERSION



Figures 10 to 15 inclusive show the effect of temperature and residence time on the main products formed.\* All products are plotted as the moles formed per mole of n-butane reacted and will be referred to as moles/mole reacted in the remainder of the discussion of results.

Carbon monoxide formed during the period of rapid reaction and then remained approximately constant at a value between 0.15 and 0.20 moles/mole reacted throughout the reactor. The carbon monoxide formation increased with increasing temperature for a given inlet oxygen concentration for most of the experimental runs. The run at 681°F, shown in Figure 10, is high, probably due to inaccuracies in the analysis at low oxygen and n-butane conversions.

Carbon dioxide formation reached a maximum in moles/mole reacted at residence times between 0.2 and 0.5 seconds, depending on the inlet temperature. The concentration of carbon dioxide decreased after reaching the maximum value to a final value of between 0.10 and 0.20 moles/mole reacted at the exit. The maximum value corresponded to the end of the induction period as indicated by the temperature profiles. The maximum carbon dioxide formation occurred probably because the oxygen concentration was close to the inlet value in the induction zone and, as the reaction started, part of the n-butane was oxidized completely to carbon dioxide and water. As more n-butane reacted, other products were formed and the overall formation of the carbon dioxide decreased.

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\* Residence times corrected for reaction conditions are described in Appendix IX.





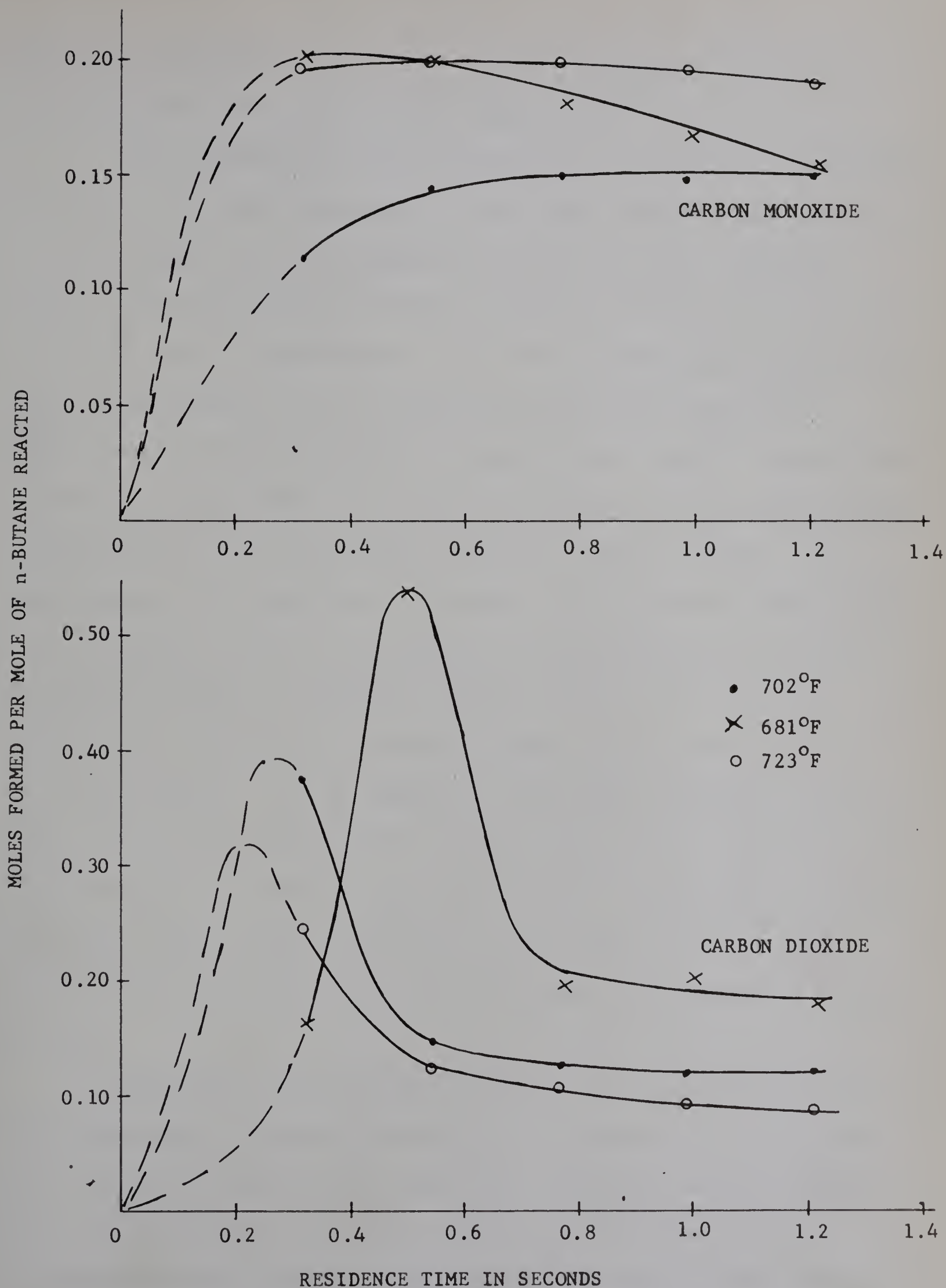


FIGURE 10: EFFECT OF TEMPERATURE ON CARBON MONOXIDE AND CARBON DIOXIDE FORMATION



The final concentration of the carbon dioxide at the reactor exit decreased with increasing temperature.

The formation of hydrogen, methane and ethane, indicated in Figure 11, were dependent on the inlet temperature mainly to the extent that the temperature affected the induction period. The formation of each increased slightly with an increase in inlet temperature. An overall effect of temperature could be determined only if the reaction was studied at a wider range of temperatures. At the reactor exit, the average hydrogen concentration was 0.05 moles/mole reacted, the methane concentration 0.15 moles/mole reacted, and the ethane concentrations 0.12 moles/mole reacted. The hydrogen composition was inaccurate due to the method of chromatographic analysis. Helium was used as a carrier gas and, as it has a thermal conductivity similar to hydrogen, gave a very poor peak on the chromatogram. As an example, 5 per cent hydrogen in air gave a peak only about 5 per cent of the recorder scale at an attenuation of 1 while 5 per cent of air, or any other similar component, gave a peak at least 50 per cent of the recorder scale at an attenuation of 4 with at least 100 times as large an area.

Ethylene and propylene formation, given in Figure 12, were important. Ethylene formed to the extent of 0.30 moles/mole reacted at the reactor exit and propylene concentration was 0.35 moles/mole reacted. Ethylene formation showed a maximum for some runs, particularly at the lower temperatures.





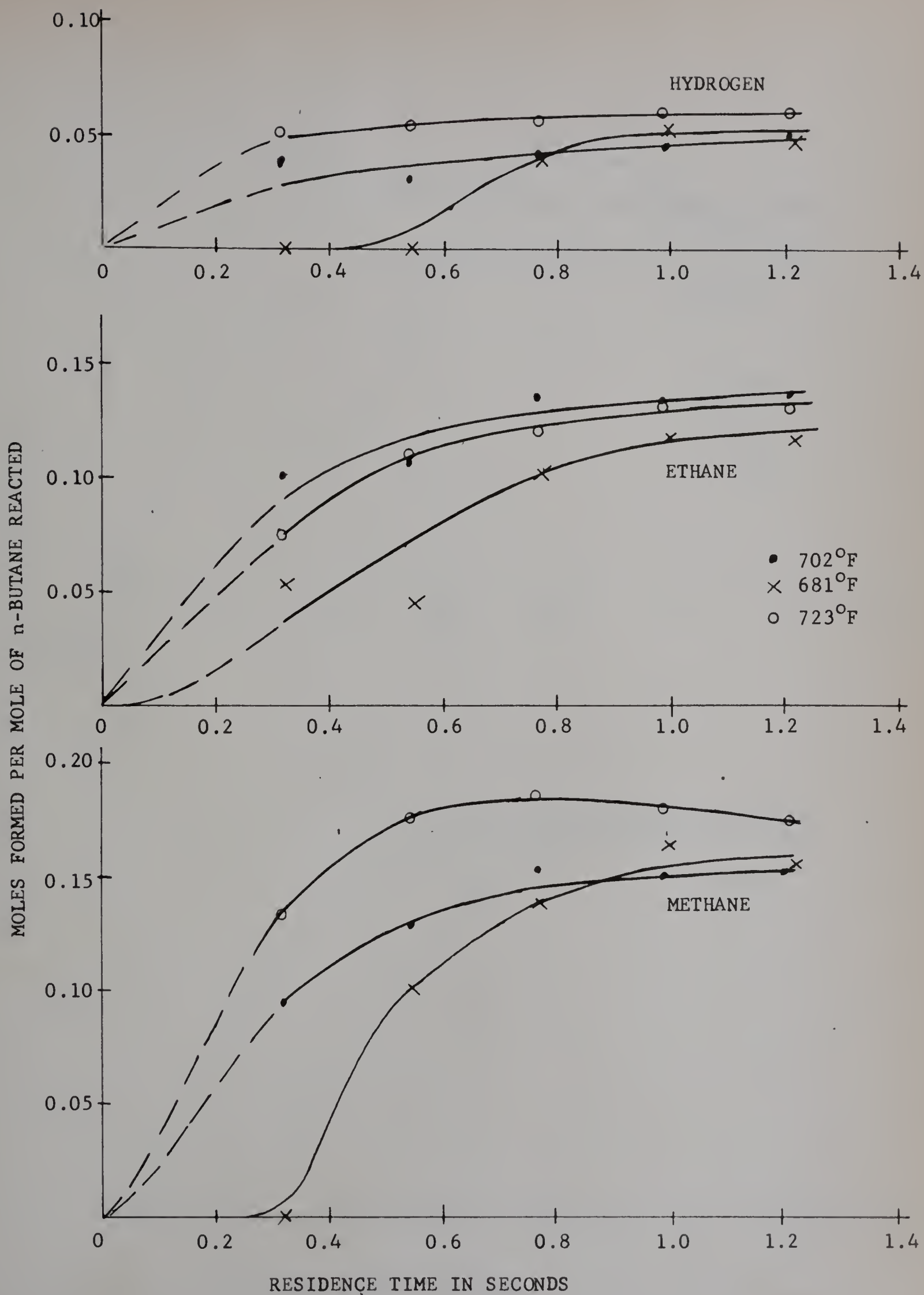


FIGURE 11: EFFECT OF TEMPERATURE ON HYDROGEN, METHANE AND ETHANE FORMATION



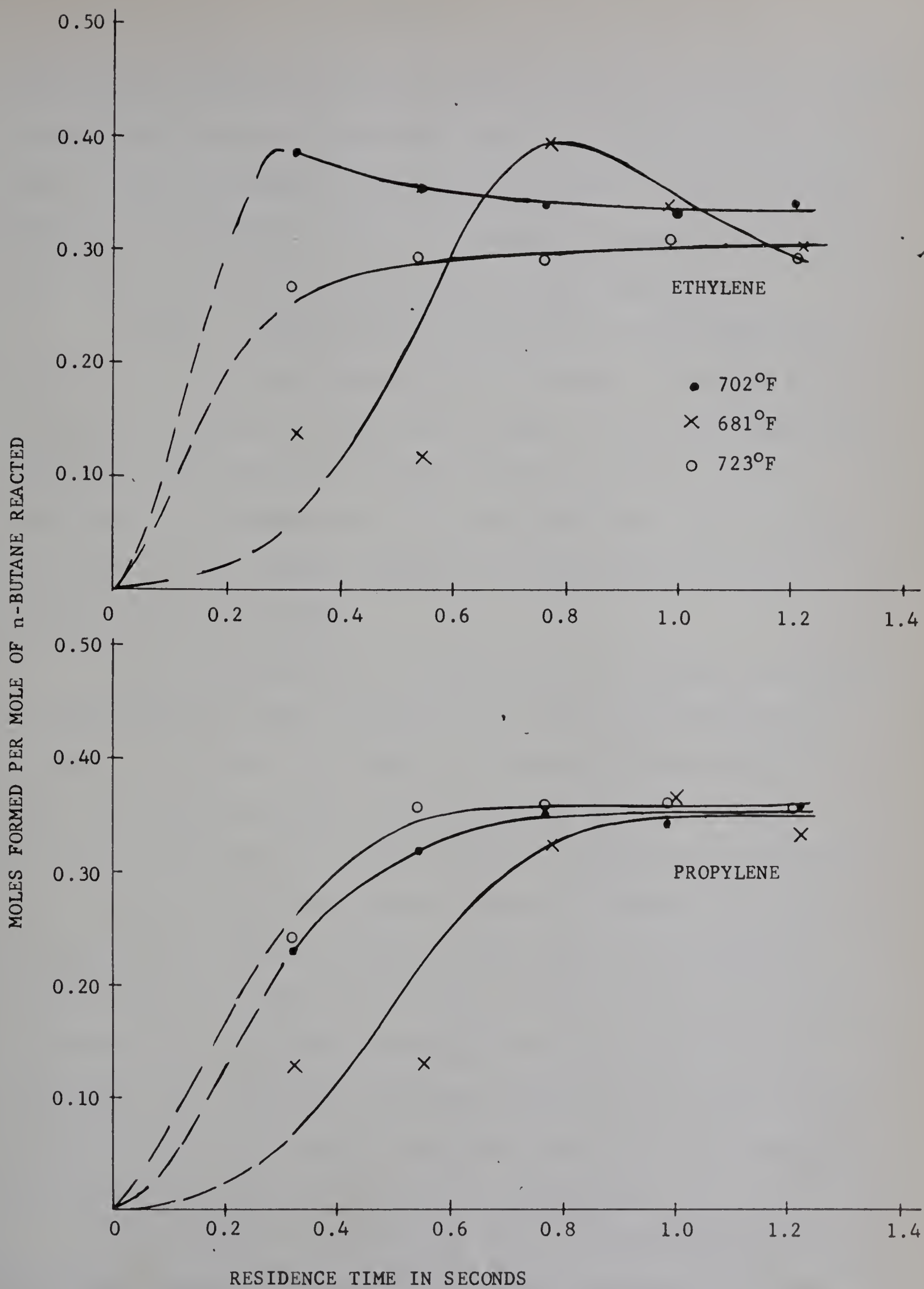


FIGURE 12: EFFECT OF TEMPERATURE ON ETHYLENE AND PROPYLENE FORMATION





The maximum formation did not always occur in the runs at 725°F. The maximum formation indicated that the ethylene reacted further or was not formed in the latter stages of the reaction. Presence of ethylene oxide in the products reported indicated that ethylene reacted with oxygen to form the oxide.

Figure 13 describes the formation of 1-butene and 2-butene in the partial oxidation of n-butane. The high formation of the butenes in the early stages of the reaction indicated that they were two of the initial products formed. Skrivan(40) and Zeelenberg and Beckel(46) both found butenes to be two of the initial products as explained by the reactions given by Skrivan.

The concentrations of 1-butene and 2-butene decreased as the residence time increased to a final concentration at the exit of between 0.10 and 0.12 moles/mole reacted for each. The concentration of the butenes was independent of inlet temperature over the range of temperatures studied.

The aldehyde and ketone formation, shown in Figure 14, was high at low residence times which indicated products formed in the initiation reactions. Once again, this was in agreement with the work of Skrivan(40) and Zeelenberg and Bickel(46) for aldehydes. Skrivan reported no ketones in the reaction system but ketones have been identified as decomposition products by Norikov and co-workers(30).

The aldehydes were mainly formaldehyde and acetaldehyde but detectable amounts of propionaldehyde and



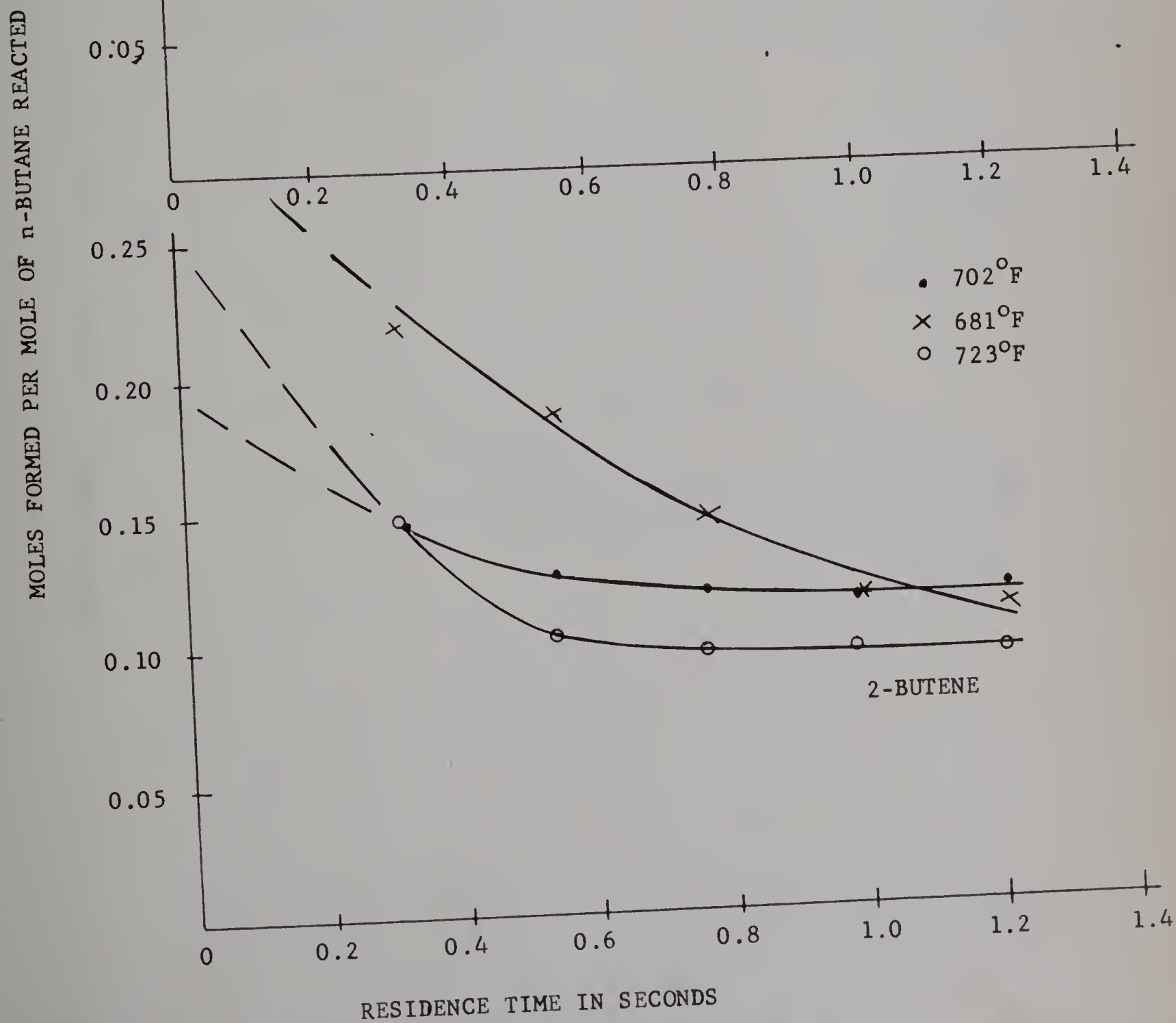


FIGURE 13: EFFECT OF TEMPERATURE ON 1-BUTENE AND 2-BUTENE FORMATION





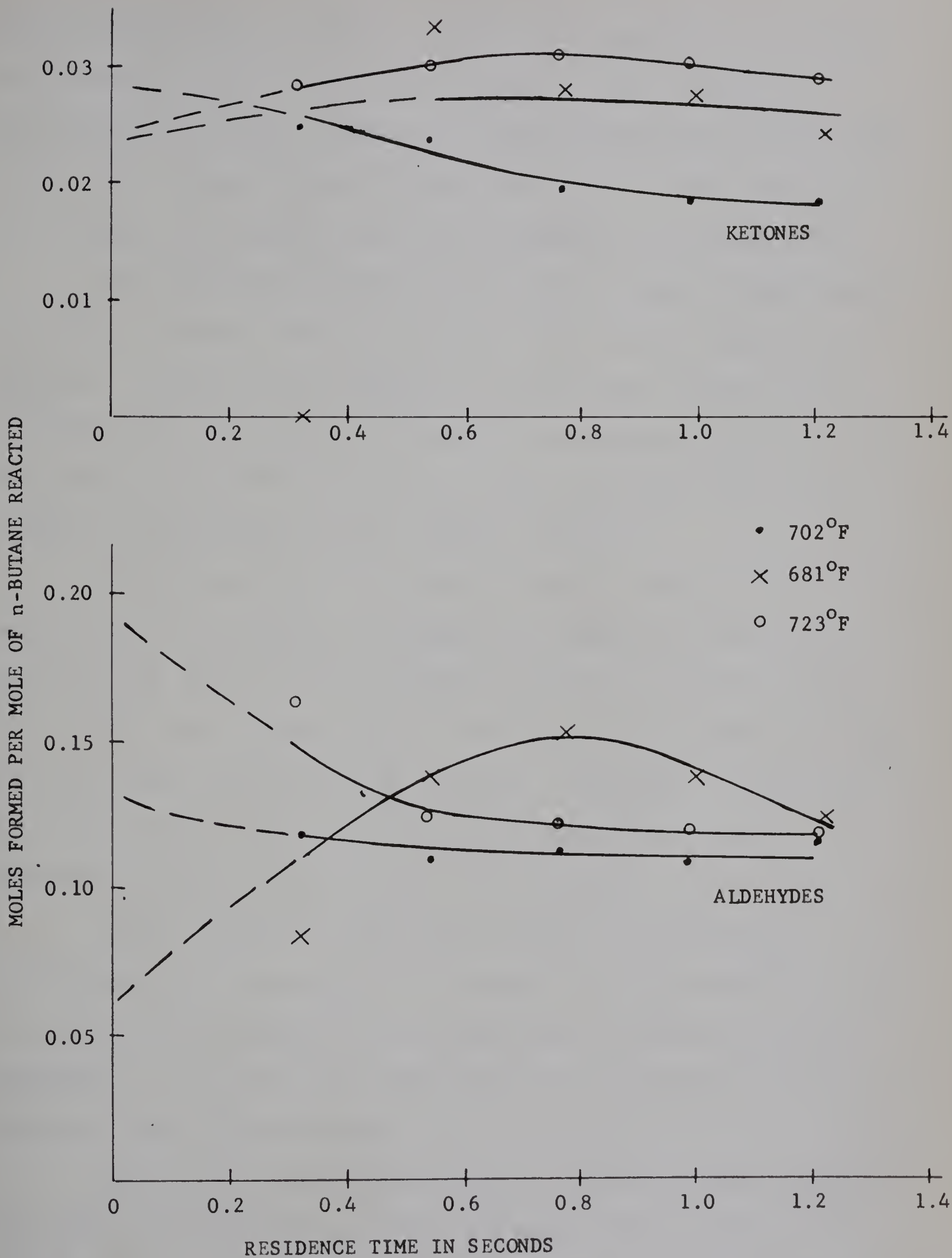


FIGURE 14: EFFECT OF TEMPERATURE ON KETONES AND ALDEHYDES FORMATION



butyraldehyde were present. Much of the decrease in aldehyde concentration with increasing residence time was due to decomposition of the aldehyde to a hydrocarbon and carbon monoxide. The concentration of the aldehydes at the exit was 0.12 moles/mole reacted and was independent of temperature.

The ketones present in the reaction system were mainly acetone and methyl ethyl ketone but some diethyl ketone was present. Ketones were formed to a much lesser degree than aldehydes and their final concentration was only 0.02 to 0.03 moles/mole reacted. No definite trend was noted as to the effect of temperature on the ketone formation.

The formation of alcohols, given in Figure 15, increased as the reaction proceeded to a value at the exit of between 0.06 and 0.10 moles/mole reacted. The alcohol analysis for the experimental run at 702°F are questionable as they are much lower than all other values. The major alcohol present was ethanol with smaller amounts of methanol and n-propanol and occasional traces of sec-butanol.

Water formation increased during the period of rapid reaction to values at the reactor exit between 0.10 and 0.15 moles/mole reacted. The final water concentration was dependent on the reaction temperature and increased with increasing inlet temperatures.

The first sample in the run at 723°F had high alcohol and water concentrations. This was detected in some of the other runs and was probably due to analysis errors.





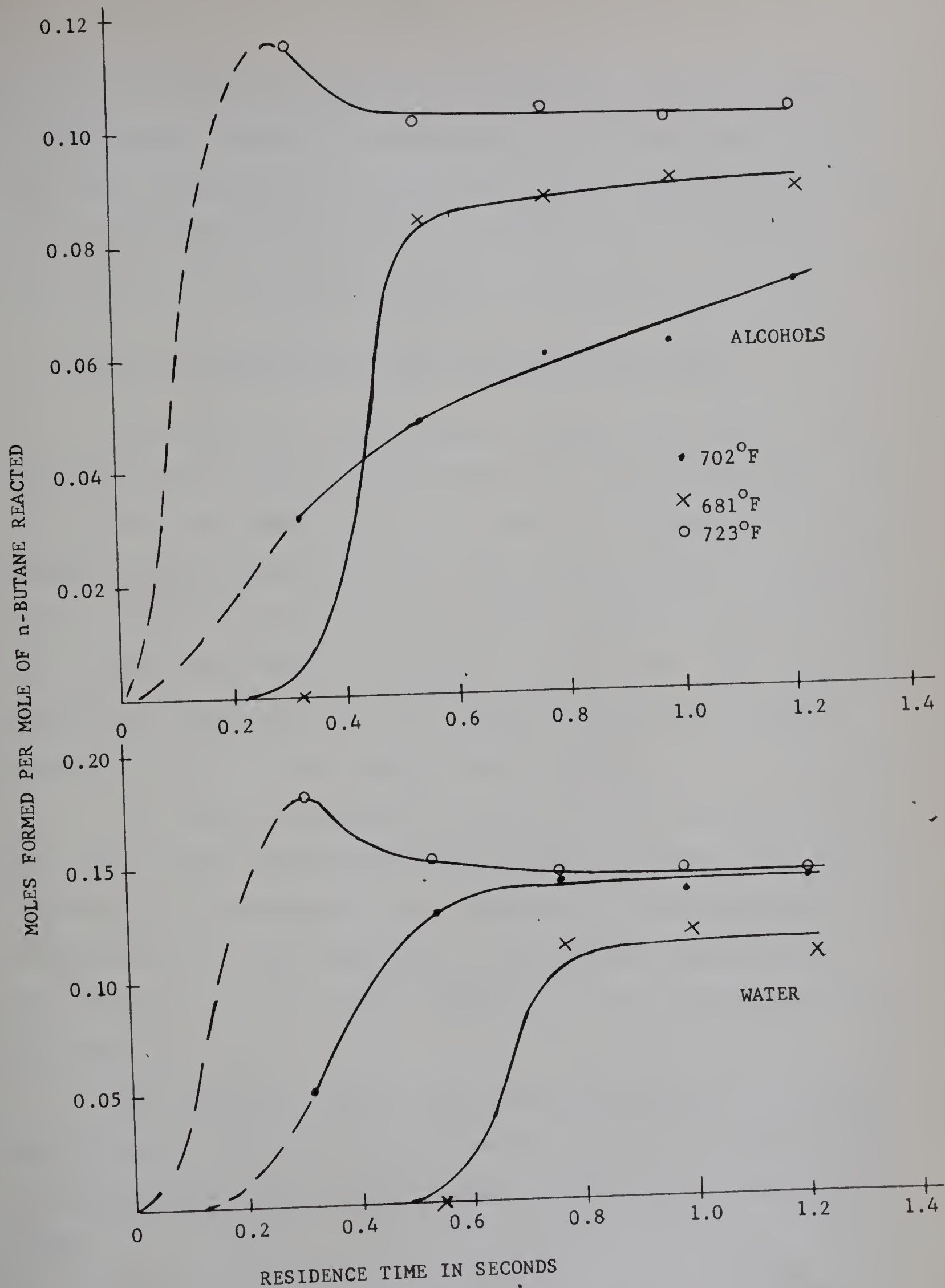


FIGURE 15: EFFECT OF TEMPERATURE ON ALCOHOLS AND WATER FORMATION



It has been impossible to present a complete picture on the overall effect of temperature on the reaction because data was not available at sufficient inlet temperatures. The large temperature rise during the period of rapid reaction interfered with the overall effect of temperature.

F. Effect of Oxygen Concentration on the Reaction

The effect of inlet oxygen concentration on the temperature profile is given in Figure 16. The experimental runs used in the plots are 11, 13, 16, and 26 at respective inlet oxygen concentrations of 6.35, 6.49, 7.25, and 8.12 mole per cent. Increased oxygen concentration caused an increase in the maximum temperature obtained in the reactor. The induction period, as determined from the temperature profile, was independent of the inlet oxygen concentrations.

The oxygen conversion is constant at 95 per cent for all inlet oxygen concentrations as shown in Figure 17. The differences in residence times required to reach the maximum conversion were not a function of the oxygen concentration but a function of the inlet temperature which varied slightly for each run.

The overall n-butane conversion increased with oxygen concentration from about 20 per cent at the low concentrations to almost 30 per cent at the higher inlet oxygen concentrations.





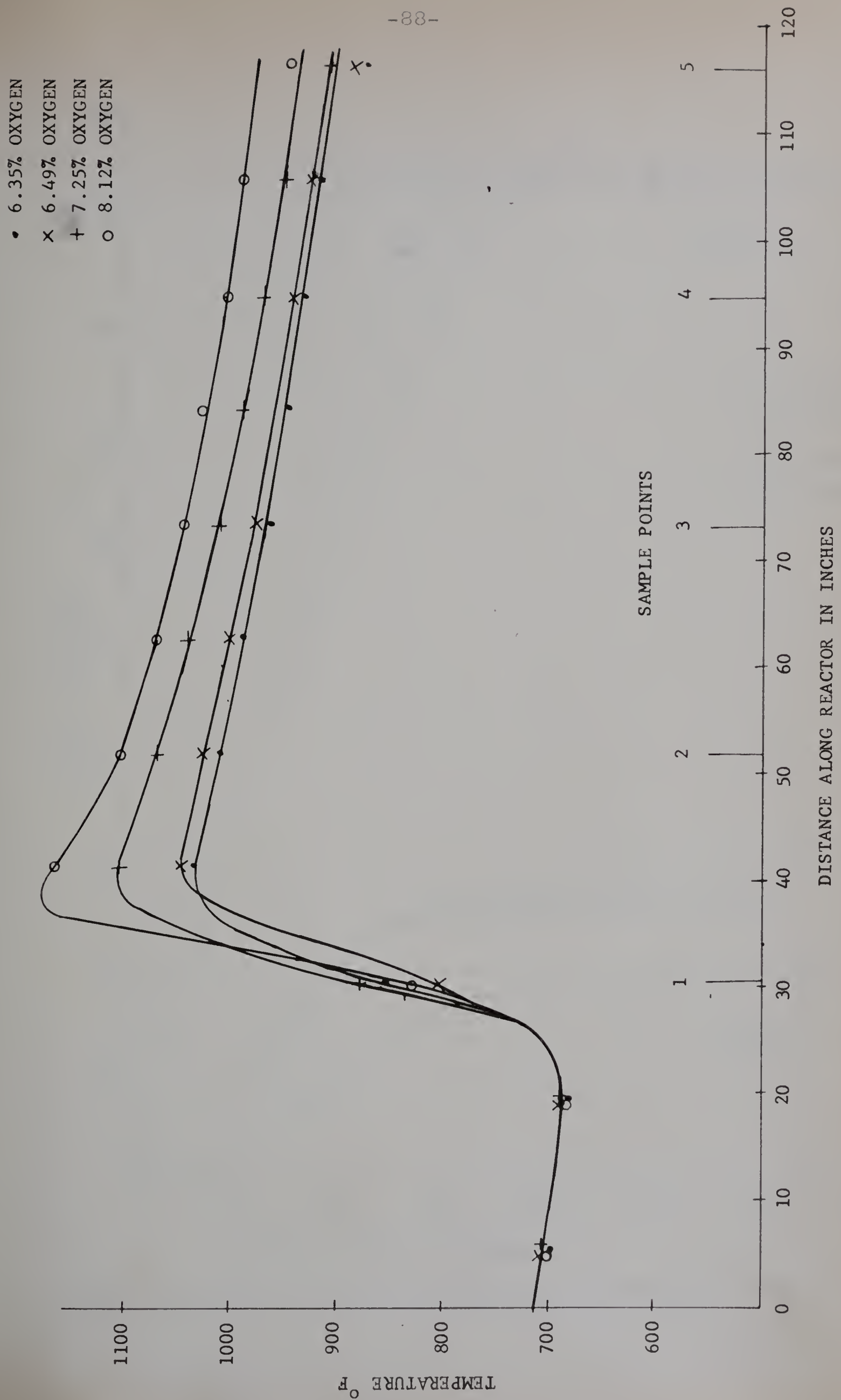


FIGURE 16: REACTION TEMPERATURE PROFILE - EFFECT OF OXYGEN CONCENTRATION



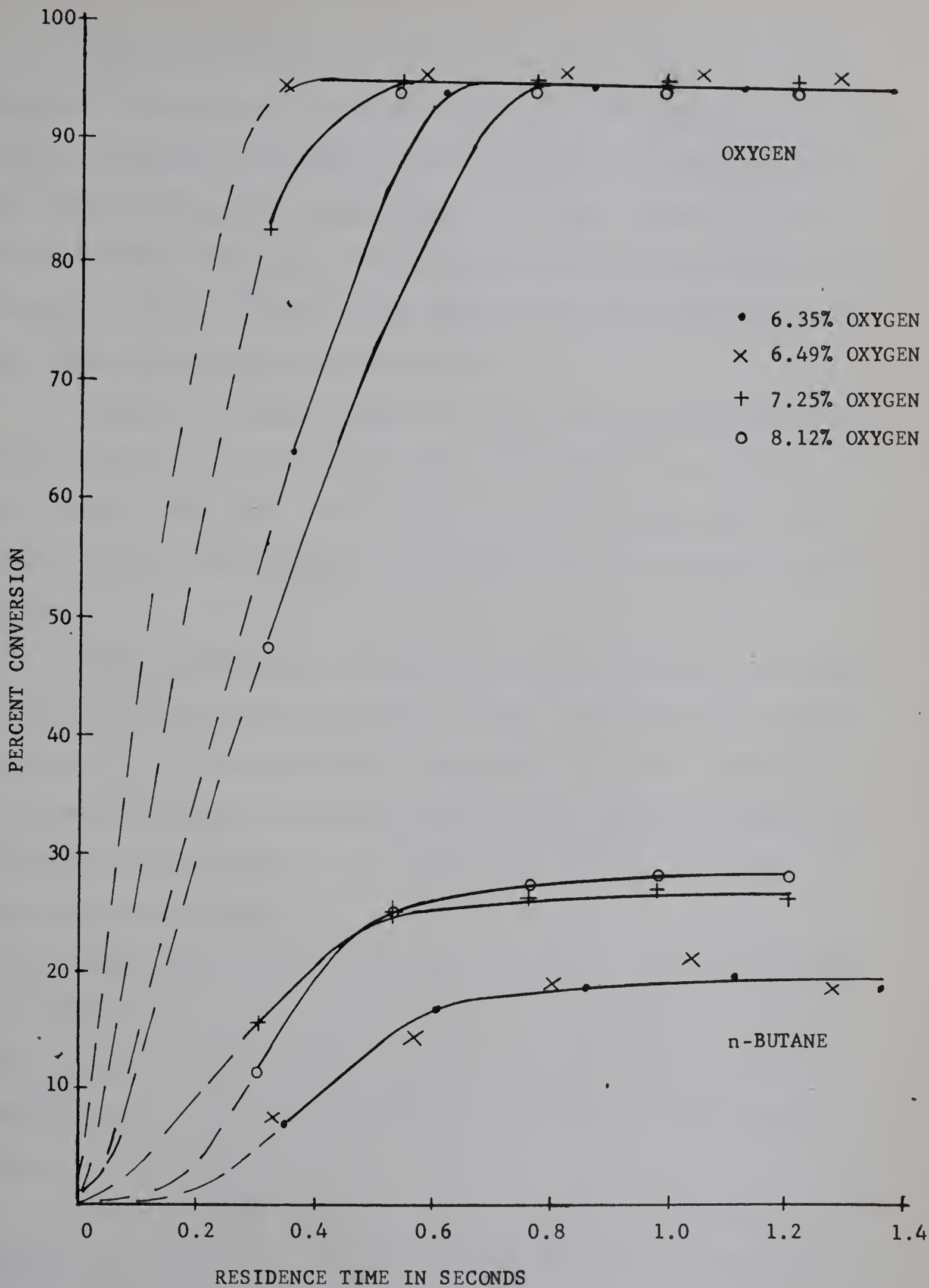


FIGURE 17: EFFECT OF OXYGEN CONCENTRATION ON CONVERSION





The moles/mole reacted for each component that was important are plotted in Figure 18 to 23 inclusive. For many of the components formed, trends could not be determined for the effect of oxygen concentration and only those of significance will be discussed. The effect of residence time on the formation of the products was discussed previously and will only be mentioned when significant.

Carbon monoxide formation was only slightly dependent on the oxygen concentration. The concentration at the reactor exit varied from 0.15 to 0.18 moles/mole reacted when the inlet oxygen concentration increased from 6.35 to 8.12 mole per cent.

Carbon dioxide formation increased with an increase in inlet oxygen concentration. At the reactor exit, the concentration of carbon dioxide increased from 0.06 to 0.15 moles/mole reacted. Carbon dioxide concentrations were a maximum in the reactor at a point just following the end of the induction period.

The formation of hydrogen, methane, and ethane were all independent of the inlet oxygen concentration over the range studied. The actual concentration of each component varied from run to run but not as a function of the inlet oxygen concentration.

On the basis of the range of oxygen concentration studied the amount of ethylene formed remained a constant.



The concentration of propylene increased slightly with an increase in oxygen concentration. The increase was very slight, however, and may have been due to analysis rather than oxygen concentration.

The formation of 1-butene and 2-butene were not affected significantly over the range of oxygen concentrations studied. The concentration of 1-butene varied between 0.10 and 0.13 moles/mole reacted at the exit while that of the 2-butene varied between 0.09 and 0.11 moles/mole reacted.

The formation of the aldehydes decreased with increasing oxygen concentration while the formation of ketones increased. At the reactor exit the aldehyde content varied between 0.17 moles/mole reacted for 6.35 mole per cent oxygen to 0.07 moles/mole reacted for 8.12 per cent oxygen. Part of this decreased formation of aldehydes was due to the chromatograph column used for the analysis of the oxygenated products. As the column was used, the separation of n-butane from formaldehyde became poorer and errors were introduced into the formaldehyde analysis. This did not account for all of the effect shown but did influence it somewhat. The ketone formation increased from 0.02 to 0.03 moles/mole reacted as the inlet oxygen concentration increased.

Alcohol formation increased with the increase in oxygen concentration from 0.07 to 0.10 moles/mole formed. The run at 7.25 per cent inlet oxygen concentration was question-





able with respect to the alcohol analysis as mentioned earlier when the effect of temperature was being discussed.

The effect of oxygen concentration on the extent of the water formation was very inconclusive. More data and better water analyses are required before the effect of reaction variables on the water content can be studied.

#### G. Reaction Mechanism

A study of the important reactions was complicated by the increase in temperature as the reaction proceeded. The increased temperature caused a decrease in the importance of the peroxide radical reactions and increased the importance of the cracking reactions as previously reported by Kalvinskas (18).

The reaction products identified by gas chromatography were explained, with a few exceptions, by the reaction scheme proposed by Skriivan(40). The plots of the moles of product formed per mole of n-butane reacted as a function of residence time in the reactor showed that butenes, aldehydes, and ketones were the initial products formed and that all other products were formed by secondary reactions. This was in agreement with Skriivan's proposal that all the products formed were dependent, either directly or indirectly, on the path of the butyl radical.

Ketones, not reported by Skriivan(40), are explained by the isomerization or decomposition reactions of the hydroperoxide radical to aldehydes or ketones. Aldehydes are pre-



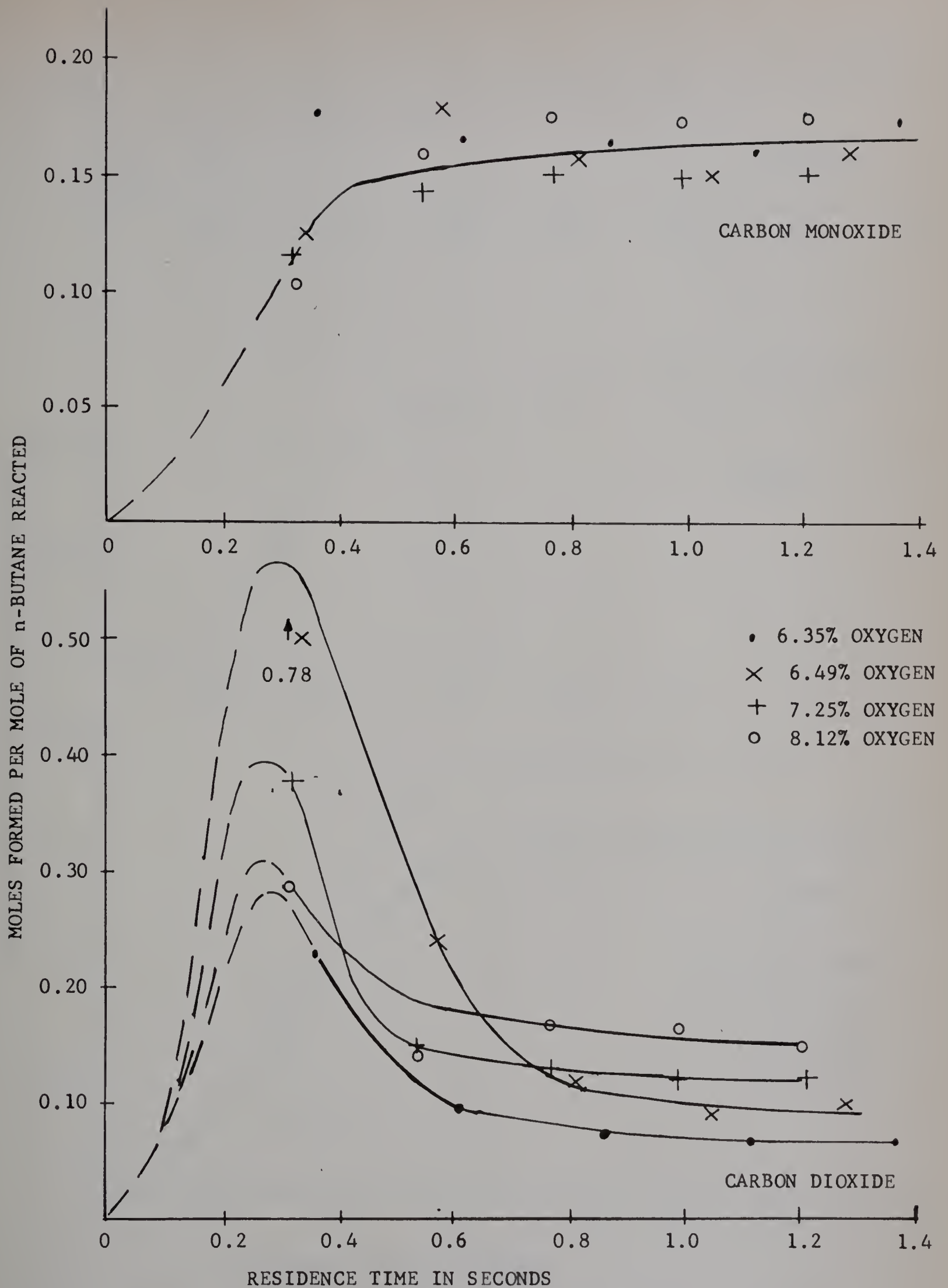


FIGURE 18: EFFECT OF OXYGEN CONCENTRATION ON CARBON MONOXIDE AND CARBON DIOXIDE FORMATION





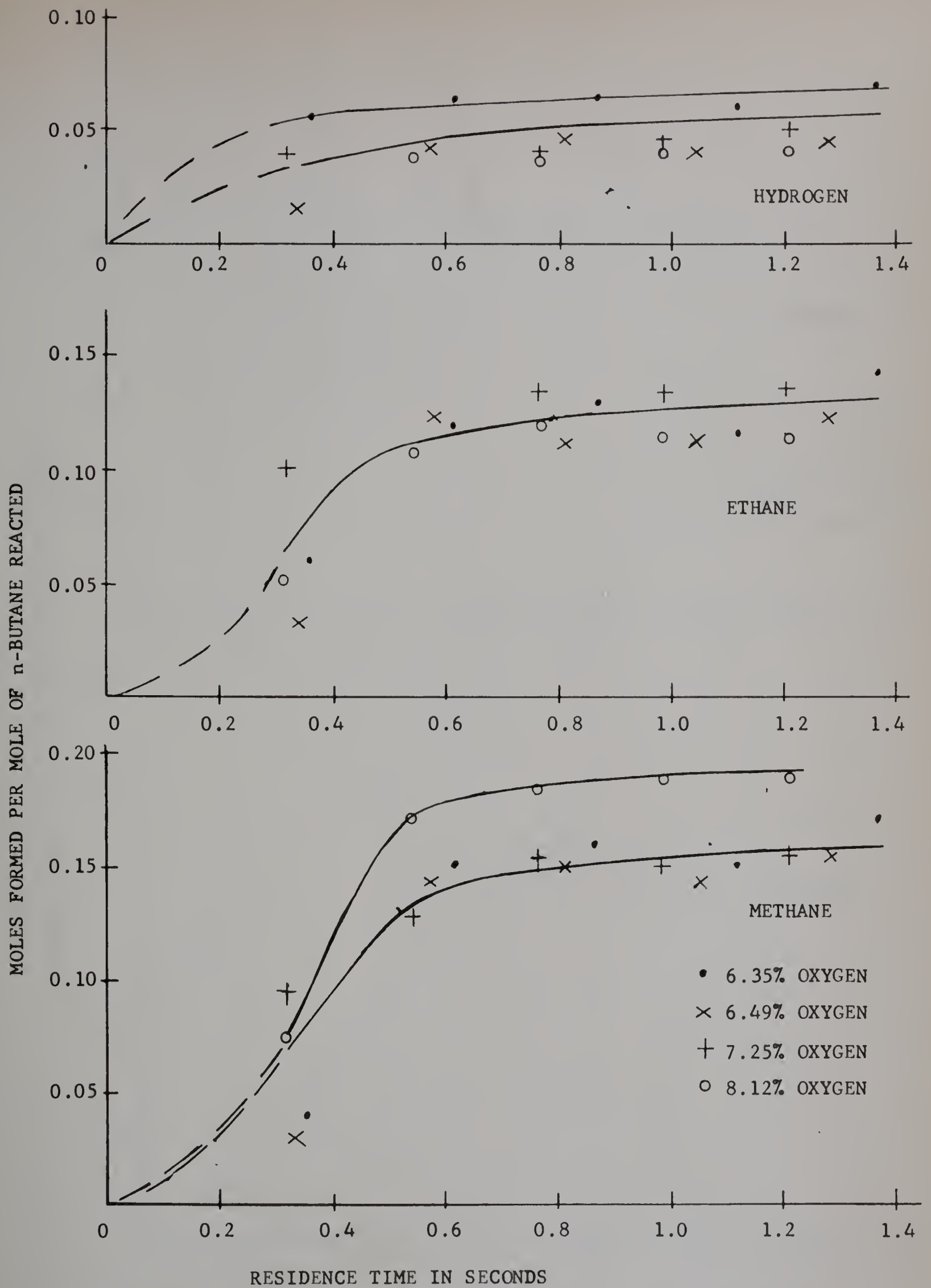


FIGURE 19: EFFECT OF OXYGEN CONCENTRATION ON HYDROGEN, METHANE AND ETHANE FORMATION



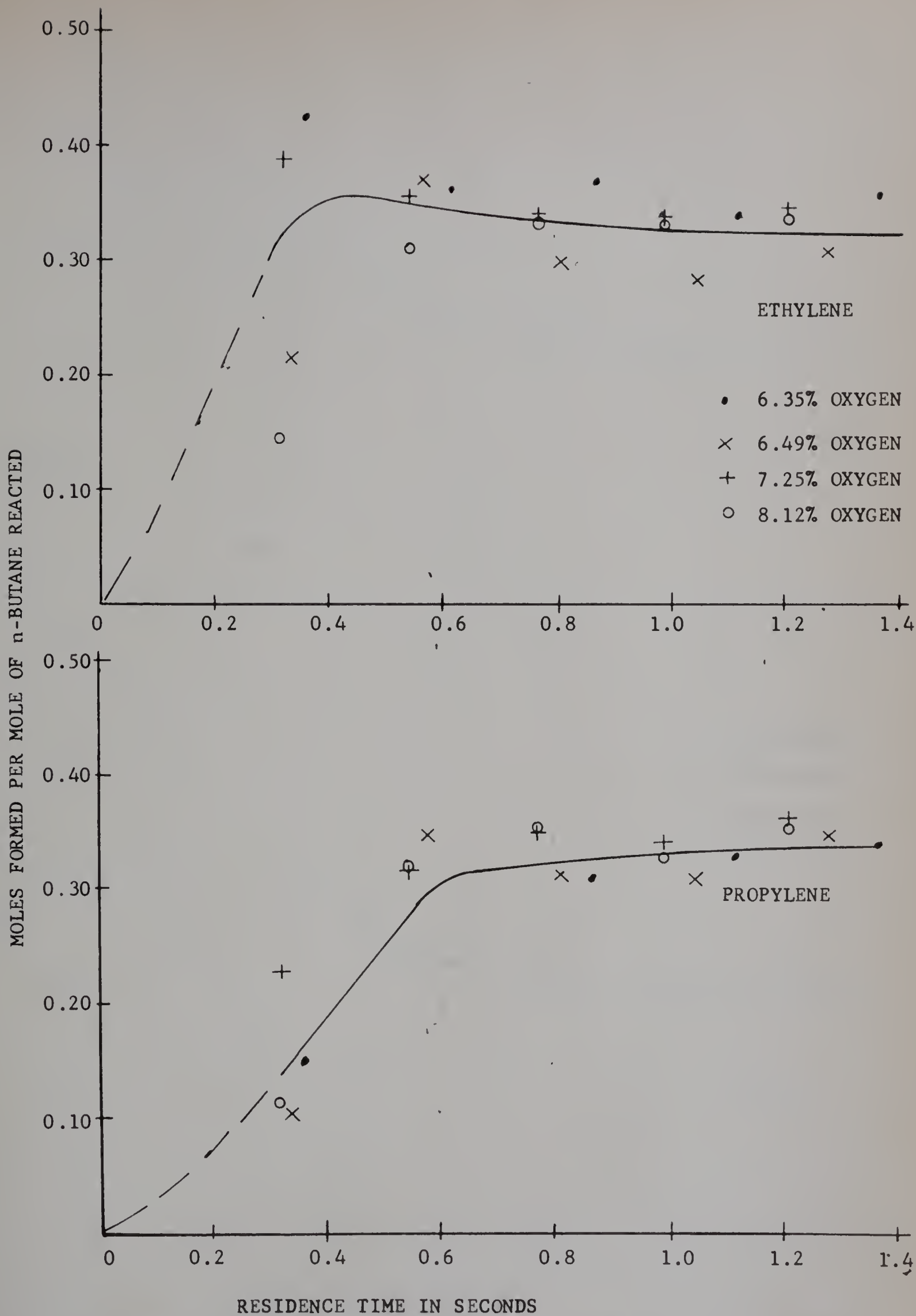


FIGURE 20: EFFECT OF OXYGEN CONCENTRATION ON ETHYLENE AND PROPYLENE FORMATION



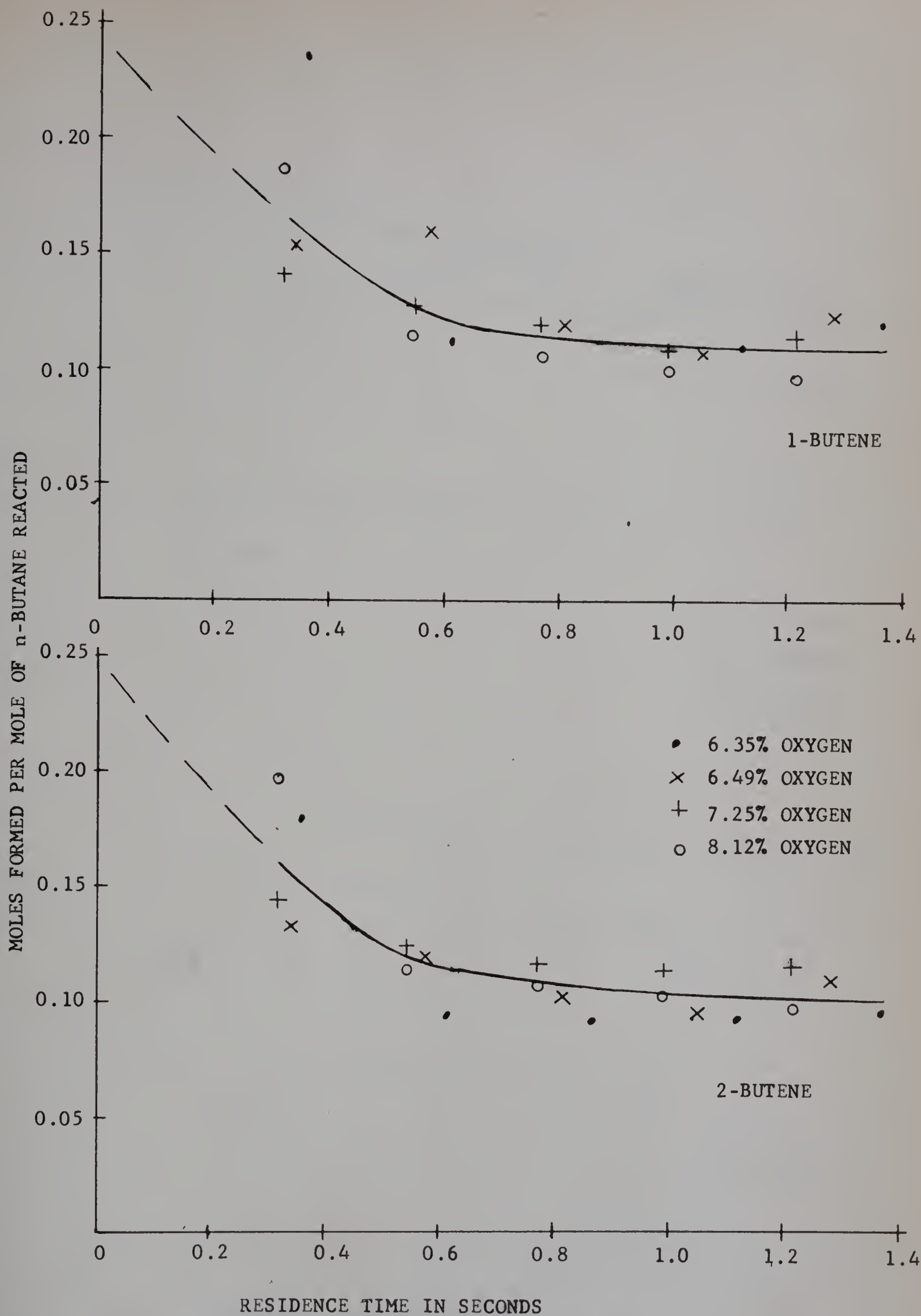


FIGURE 21: EFFECT OF OXYGEN CONCENTRATION ON 1-BUTENE AND 2-BUTENE FORMATION





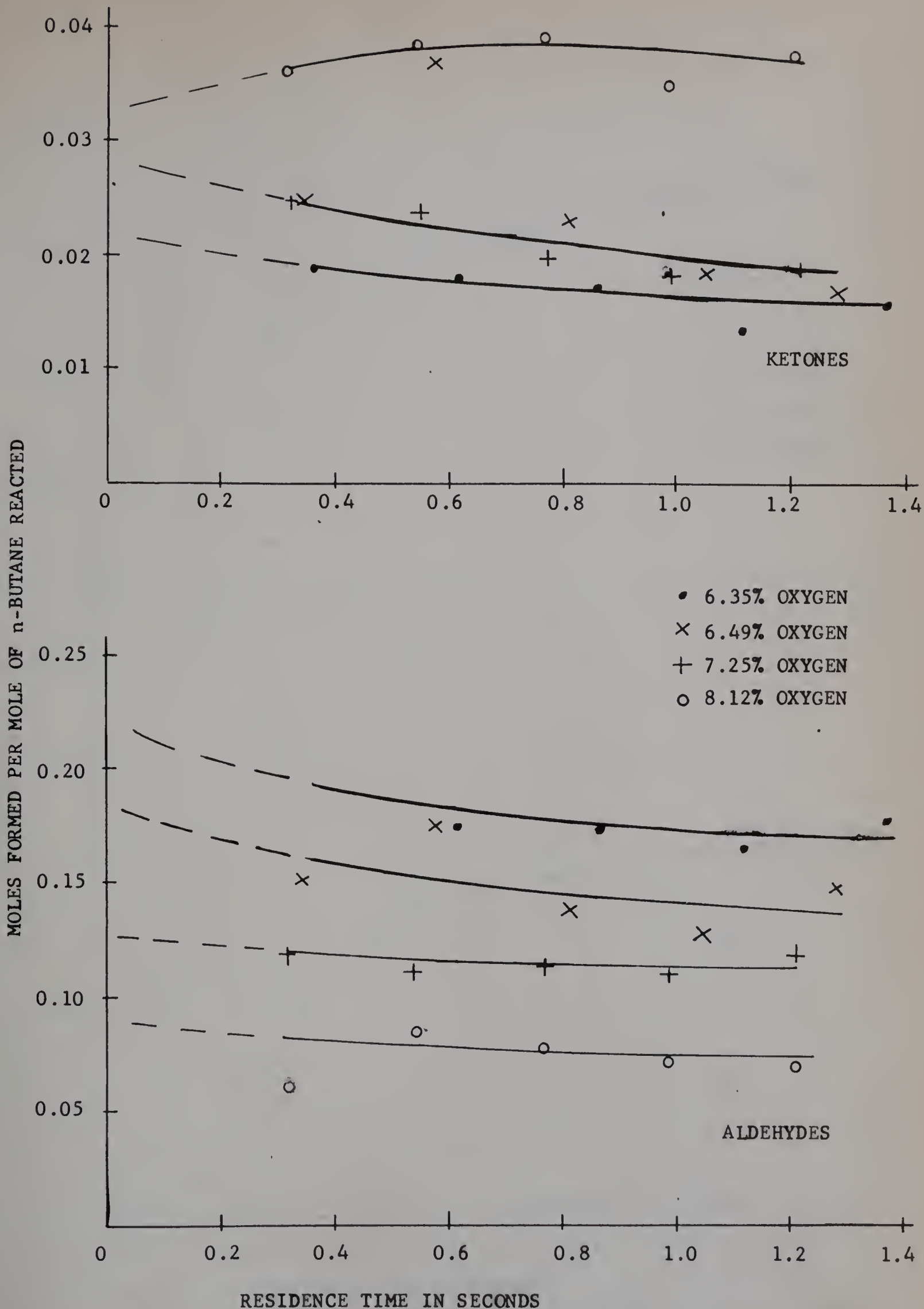


FIGURE 22: EFFECT OF OXYGEN CONCENTRATION ON ALDEHYDES AND KETONES FORMATION



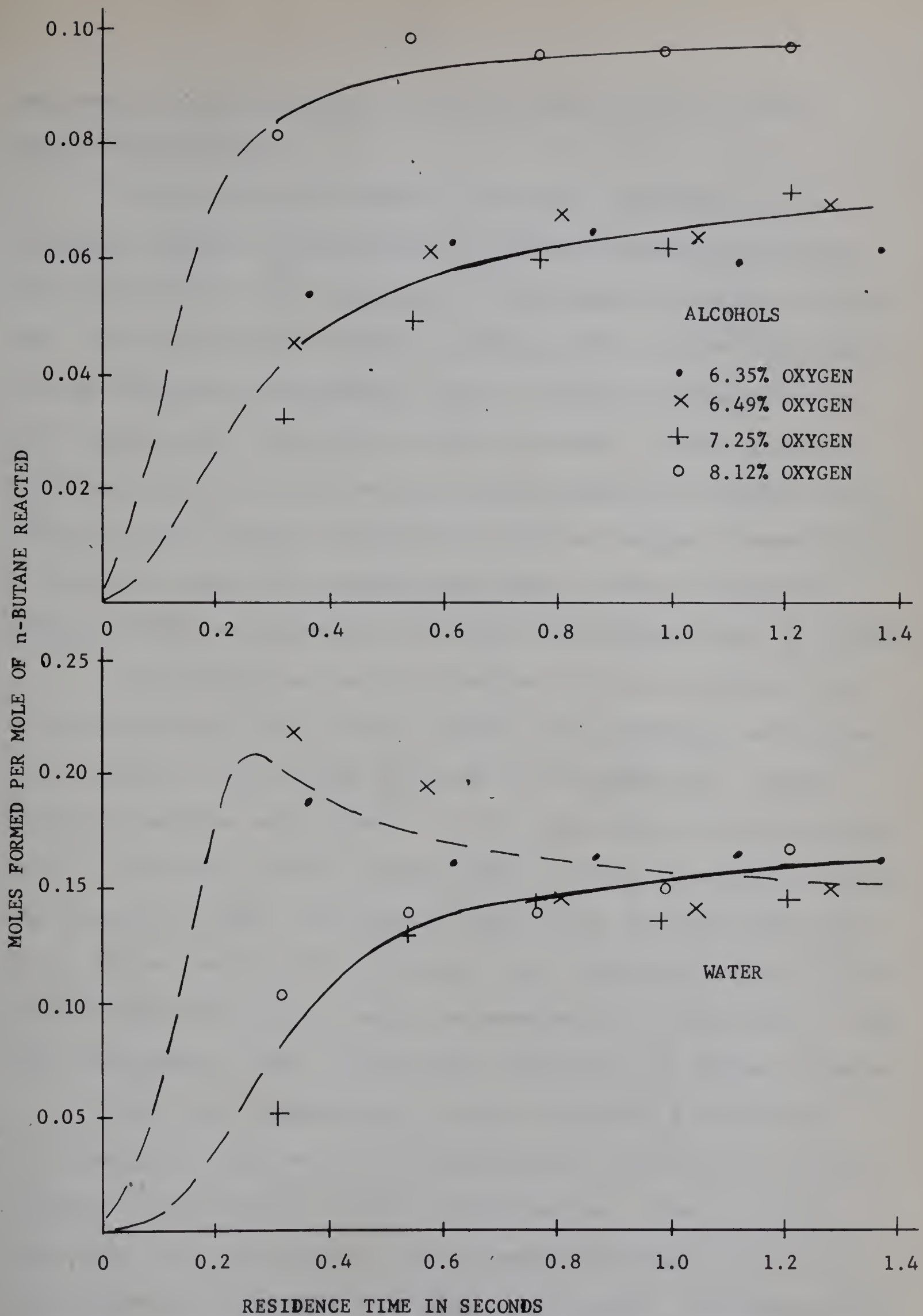


FIGURE 23: EFFECT OF OXYGEN CONCENTRATION ON ALCOHOLS AND WATER FORMATION





dominant in the decomposition reactions because of lower energy requirements.

Carbon dioxide formation was not explained by the reaction schemes of Skrivan(40) or Kalvinskas(18) although both research workers reported its presence in product analyses. The high carbon dioxide concentration at the beginning of the reaction was probably due to complete oxidation of a small amount of n-butane to carbon dioxide. Later in the reaction carbon dioxide was no longer formed by complete oxidation of the n-butane because of the low oxygen concentration. At the high reaction temperatures used, carbon dioxide was formed by the decomposition of acids to hydrocarbons or ketones.

An attempt was made to derive a rate expression for the rate of reaction of the n-butane and, although unsuccessful, several variables were found to be important. Three distinct periods were present in all experimental runs including the induction period during which little reaction occurred, the period of rapid reaction in which most of the oxygen and 20 to 30 per cent of the n-butane were consumed, and the final period where secondary reactions occurred at a slow rate. Any rate expressions must incorporate terms for all these periods.

The inlet temperature to the reactor is important as it controls the length of the induction period and has an effect on the overall product distribution. Thus, a term which includes the reactor inlet temperature must be in the rate expression to cover the induction period. Although they were not studied in this research program, other variables



have been found by Dalla Lana(9), Musgrove(27) and others which affect the length of the induction period. These variables include flow conditions in the reactor, surface area to volume ratio, and reactor wall surface. The effect of these variables on the induction period must be studied further before they can be incorporated into the rate expression for the induction period.

The reaction temperature is of importance as it has an effect on the rate constant as given by the Arrhenius equation(43),

$$k = A e^{-E/RT}$$

where

k = reaction rate constant

A = Arrhenius constant for the reaction

E = activation energy

R = gas constant

T = absolute temperature

Kalvinskas(18), Shtern(39), and others have reported a negative temperature coefficient for the partial oxidation reaction which must be considered in the derivation of an overall rate of reaction. The negative temperature coefficient occurs at intermediate temperatures at which the peroxide radical reactions have ceased to be important due to instability of the peroxide radicals and the cracking reactions have slow rates due to the low temperature.





The rate of butane reaction is dependent on the concentration of both oxygen and butane in the system and both must be considered in any rate expression. The dependence on the oxygen concentration has been shown in all of the experimental runs as indicated by the slow reaction rate after the major portion of the oxygen had been consumed. Proof that the reaction rate is dependent on the n-butane concentration has not been determined conclusively in the present program but has been previously shown by Kalvinskaskas(18). The present experimental runs demonstrate the n-butane effect on the reaction only by showing that the n-butane reacts even after the major portion of the oxygen has been consumed, although at a much slower rate.

No attempt was made to compare to present data with rate expressions derived by Skrivankas(40) and Kalvinskaskas(18) because of limitations on the use of these rate expressions. Skrivankas's rate expression was derived from data that showed no induction period in the reactor, and as a result, included no term for the induction period. This suggests that his rate expression has only limited applicability and certainly cannot fit the present data. Kalvinskaskas derived his rate expression for a reaction scheme that showed only hydrocarbons in the product with no oxygenated products, except water, being present. No comparison was made using the present data as the reaction scheme used by Kalvinskaskas certainly does not describe the present system.





## H. Heat of Reaction

The heat of reaction for run number 16 was calculated by two methods and the results were compared. The overall heat of reaction was calculated using the heats of formation of the reactants and products for the exit gas stream at 77°F and corrected to the reaction temperature of 702°F by means of the specific heat values for each component.

$$\Delta H_R)_{77^\circ\text{F}} = \sum \Delta H_F)_{\text{PROD.}} - \sum \Delta H_F)_{\text{REACT.}}$$

$$\Delta H_R)_{702^\circ\text{F}} = \Delta H_R)_{77^\circ\text{F}} + \int_{77}^{702} \Delta C_p \, dT$$

where

$$\Delta H_R)_{77^\circ\text{F}} = \text{heat of reaction at } 77^\circ\text{F}$$

$$\Delta H_R)_{702^\circ\text{F}} = \text{heat of reaction at } 702^\circ\text{F}$$

$$\Delta H_F)_{\text{PROD}} = \text{heat of formation of products at } 77^\circ\text{F}$$

$$\Delta H_F)_{\text{REACT}} = \text{heat of formation of reactants at } 77^\circ\text{F}$$

$$\Delta C_p = C_p)_{\text{PROD}} - C_p)_{\text{REACT}}$$

= heat capacity difference between  
products and reactants

$$T = \text{absolute temperature}$$

The overall heat of reaction was calculated to be -26,400 BTU/lb.mole of n-butane reacted. The heat release, defined as the amount of heat produced by the reaction per hour, was calculated from the heat of reaction and the reactant flow rate to be 8,380 BTU/hr.



The rate of heat release was also calculated from the increase in temperature of the gas stream and the heat transferred from the gas to the reactor wall by the equation

$$Q = h A_i (T_G - T_w) + w C_{p_{AV}} (T_F - T_O)$$

where

$Q$  = heat released BTU/hr

$h$  = heat transfer coefficient from the gas to the reactor wall

$A_i$  = reactor surface area

$T_G$  = gas temperature

$T_w$  = reactor wall temperature

$w$  = weight rate of flow through the reactor

$C_{p_{AV}}$  = average specific heat of gases

$T_F$  = exit temperature of gas stream

$T_O$  = inlet temperature of gas stream

The rate of heat release was found to be 6800 BTU/hr.

The differences in these answers were due mainly to the problem of calculating the heat transferred from the gas to the reactor wall. A heat transfer coefficient calculated at entrance conditions was used throughout as the effect of the reaction on the stream properties, mainly viscosity and thermal conductivity, were unknown.







## CONCLUSIONS

The reactor used in the study of the partial oxidation of n-butane functioned well in most respects for the experimental program. The control systems for the reactor were very satisfactory and maintained the reaction variables at the desired settings. The overall carbon and hydrogen balances on all the reaction samples verified the accuracy of the n-butane flow controller.

The electrical heaters for the reactor were not completely satisfactory as it was impossible to maintain a constant wall temperature, even for the runs with n-butane in which no reaction occurred. The control thermocouple for the reactor heaters was positioned poorly and, for many experimental runs, the reactor wall at the entrance was below the reaction temperature which resulted in cooling of the gases prior to the start of the reaction.

The chromatographic analysis for all components, except carbon dioxide, hydrogen, and water, was good as indicated by the carbon and hydrogen balances based on the amount of butane reacted and the overall oxygen balance. The low, and fluctuating, overall oxygen balance indicated poor carbon dioxide and water analysis and the hydrogen balance based on the butane reacted confirmed low water and hydrogen analyses. The poor carbon dioxide analysis was caused by poor separation on the chromatographic columns used. Carbon dioxide was not separated from ethylene on the Silica Gel column and had to



be determined by a difference between the ethylene and carbon dioxide peak on the Silica Gel column and the ethylene peak on the Molecular Sieve column. The poor water analysis occurred because of the poor resolution of the water peak on the Ucon column. The hydrogen analysis was low because of the low sensitivity of the chromatograph for hydrogen when helium was being used as the carrier gas.

The temperature of the gas stream increased rapidly from the inlet temperature during the period of rapid reaction to a peak temperature approximately 400°F above the inlet temperature. After the period of rapid reaction, the gas phase temperature decreased due to heat transfer to the reactor wall. Errors in the gas phase thermocouple readings are not believed to exceed 10 to 12°F. (Due to radiant and conductive heat transfer from the thermocouples to the reactor wall.)

Analysis of samples showed that on the average 60 per cent of the n-butane that reacted was converted to olefins, 10 per cent to hydrocarbons of lower molecular weight, 10 per cent to carbon oxides, and 20 per cent to oxygenated products consisting of aldehydes, ketones, and alcohols. In all the experimental runs, between 20 and 30 per cent of the butane reacted throughout the reactor. Ninety-five per cent of the oxygen was consumed by the end of the period of rapid reaction but no further conversion was detected in the reactor.

The experimental runs made at different inlet temperatures described the effect of the inlet temperature on the in-





duction period. For inlet temperatures of 685°F, the induction period lasted approximately 0.5 seconds but at 725°F, the induction period was only 0.2 seconds.

The products identified in the reaction mixtures are consistent with the reaction scheme proposed by Skrivan(40), in which the formation of all products was dependent on the path of the butyl radical. Butenes, aldehydes, and ketones were identified as the primary products formed with all others being secondary.

A study of the rate of decomposition of the n-butane showed the importance of several variables. The inlet temperature was important as it controlled the length of the induction period and affected the product distribution. Finally, n-butane and oxygen concentrations were both found to have an effect on the rate of decomposition. Any rate equation capable of describing the decomposition of n-butane in a partial oxidation reaction must take into account all of these variables as well as many others not studied here.





## RECOMMENDATIONS

Several features of the experimental equipment were found to cause poor temperature distribution in the reactor and, if eliminated before any future work is done, would provide better temperature control and distribution in the reactor. The reactor control thermocouple should be located at the reactor entrance in order to maintain a constant gas temperature until the rapid reaction begins.

Methods should be employed to provide a reactor wall temperature that is closer to being constant than was obtained during the present experimental program. One method would be to remove part of the insulation from the reactor wall and thereby increase the heat losses.

The reactor should be adapted for the use of solids in the gas stream to act as heat sinks for the heat of reaction. The solids would reduce the magnitude of the temperature increase without inhibiting the reaction.

The reactor exit should be insulated better so that the temperature profile and product distribution are not affected until after the sample point at the exit. At the present, the space between the bottom electrical heater and the exit flange is uninsulated. Temperatures measured in this region are lower than they should be according to the profiles obtained and could easily be corrected.

A better chromatographic analysis of the product



samples could be obtained if different columns were used for the separation of certain components. Carbon dioxide and water analyses were poor and a better choice of columns could give a better analysis. The amount of hydrogen formed should be determined either by some other means or by chromatographic analysis only if some other carrier than helium is used. Helium has a thermal conductivity very close to hydrogen and the peak for hydrogen is inaccurate.

Further work should be carried out on the equipment to determine the effect of temperature, oxygen concentration, and reactor pressure on the partial oxidation of n-butane. To study the effect of temperature, the residence time must be varied so that product samples are obtained in the induction period, the period of rapid reaction, and the final period during which little reaction takes place. The reactor should be converted so that either enriched air or pure oxygen may be used to study the effect of oxygen concentration on the reaction.







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## APPENDIX I

### THERMOCOUPLE AND SAMPLE LINE LOCATION





The thermocouple locations in the reactor are given in Table I-1. The thermocouple numbers are the numbers corresponding to the temperature recorder channels. The actual thermocouple locations are given in distances measured from the mixing point of gases in the preheater when the reactor is hot. The thermal expansion of the reactor is divided evenly over the reactor length even though it may be higher in some sections due to the higher wall temperatures. The temperature that the thermocouple measures is indicated by "G" if the thermocouple is in the gas stream, and by "W" if it is in the reactor wall. Thermocouples 1 to 15 are in the reactor and number 16 is in the preheater. The locations of the preheater and reactor control thermocouples are included in Table I-1.

Table I-2 gives the locations of the sample points. The sample point positions are reported, in the same manner as for the thermocouples, as the distance measured from the mixing point of the n-butane and air in the preheater.

All thermocouples and sample lines are located within  $\pm 0.1$  inch of the point as reported.



Table I-1Location of Thermocouples

Thermocouple Number	Location: inches From Mixing Point	Temperature Measured
1	19.7	G
2	30.4	G
3	30.4	W
4	41.1	G
5	51.8	G
6	51.8	W
7	62.5	G
8	73.2	G
9	73.2	W
10	83.9	G
11	94.6	G
12	94.6	W
13	105.3	G
14	116.0	G
15	116.0	W
16	6.0	G
Preheater	6.0	G
Reactor	51.8	G



Table I-2Location of Sample Points

Sample Line Number	Location: Inches From Mixing Point	Location: Fraction of Reactor Length
1	30.4	0.260
2	51.8	0.443
3	73.2	0.626
4	94.6	0.809
5	116.0	0.992





## APPENDIX II

RETENTION TIMES FOR THE COMPONENTS

SEPARATED BY GAS CHROMATOGRAPHY

SAMPLE CHROMATOGRAMS



The retention times for all the components separated on each column are given in Tables II-1 to II-4. Also included in these tables are the relative response factors and correction factors for all components. Correction factors are not reported for the Molecular Sieve and Molecular Sieve-Charcoal columns as these columns are operated at constant temperatures. The component numbers, given for all components, are used in Appendices VI and VII for the compounds reported in the analyses and product distributions.

Sample chromatograms are shown, one for each column used in the separation, in order to indicate the degree of separation obtained. The components separated and the attenuation for each peak are given on the chromatograms.





Table II-1

Retention Times for Components Separated  
on the Ucon Column

Component Number	Component	Retention Time Minutes	Relative Response Factor	Correction Factor
1	Hydrogen	2.8	*0.0085	1.00
2,3	Air	2.8	0.42	1.00
4	Carbon Monoxide	2.8	0.42	1.00
5	Methane	2.8	0.36	1.00
6	Ethane	3.1	0.51	1.00
7	Carbon Dioxide	3.1	0.48	1.00
8	Ethylene	3.1	0.48	1.00
9	Propane	3.8	0.65	1.00
10	Propylene	3.8	0.63	1.00
11	i-Butane	4.4	0.82	1.00
12	n-Butane	5.0	0.85	1.00
13	1-Butene	5.0	0.81	1.00
14	2-Butene	5.0	0.86	1.00
15	Formaldehyde	5.8	*0.58	1.00
16	Ethylene Oxide	6.3	0.68	1.00
17	2-Methyl Butane	7.1	1.05	1.00
18	Acetaldehyde	7.7	*0.69	1.00
19	n-Pentane	8.6	1.05	1.00
20	Propylene Oxide	9.6	0.80	1.00
21	3-Methyl Pentane	10.5	1.19	1.00
22	n-Hexane	12.7	1.23	1.00
23	Propionaldehyde	13.7	*0.80	1.00
	Unknown	14.5		
24	Acetone	15.2	0.86	1.00
25	Methanol	16.9	0.55	1.03
26	Water	17.8	0.21	1.00



Table II-1 - continued

Component Number	Component	Retention Time Minutes	Relative Response Factor	Correction Factor
	Unknown	19.5		
27	Ethanol	20.5	0.72	1.05
28	Butyraldehyde	22.1	*0.92	1.07
29	Methyl Ethyl Ketone	23.4	0.98	1.08
30	n-Propanol	29.3	0.83	1.10
31	Diethyl Ketone	30.4	1.10	1.10
	Unknown	31.7		
	Unknown	36.7		
32	sec-Butanol	39.4	0.97	1.10
	Unknown	44.0		
	Unknown	46.0		

\* Relative Response Factors for Aldehydes and Hydrogen were determined as part of the present program.



Table II-2

Retention Times for Components Separated  
on the Silica Gel Column

Component Number	Component	Retention Time Minutes	Relative Response Factor	Correction Factor
1	Hydrogen	4.8	0.0085	1.00
2,3	Air	4.8	0.42	1.00
4	Carbon Monoxide	4.8	0.42	1.00
5	Methane	4.8	0.36	1.00
6	Ethane	6.9	0.51	1.00
7	Carbon Dioxide	7.7	0.48	1.00
8	Ethylene	7.7	0.48	1.00
9	Propane	10.4	0.65	1.00
10	Propylene	14.1	0.63	1.00
11	i-Butane	17.0	0.82	1.00
12	n-Butane	17.0	0.85	1.00
13	1-Butene	22.5	0.81	1.02
14	2-Butene	25.1	0.86	1.03





Table II-3

Retention Times for Components Separated  
On the Molecular Sieve Column

Component Number	Component	Retention Time Minutes	Relative Response Factors
1	Hydrogen	1.5	0.0058
2,3	Air	1.5	0.42
4	Carbon Monoxide	1.8	0.42
5	Methane	1.8	0.36
6	Ethane	4.7	0.51
8	Ethylene	9.0	0.48

Table II-4

Retention Times for Components Separated  
on the Molecular Sieve-Charcoal Column

Component Number	Component	Retention Time Minutes	Relative Response Factors
1	Hydrogen	2.4	0.0085
2	Oxygen	5.7	0.40
3	Nitrogen	6.4	0.42
4	Carbon Monoxide	9.3	0.42
5	Methane	19.8	0.36

10

PROPYLENE OXIDE

3-METHYL PENTANE

n-HEXANE

PROFIONALDEHYDE

15

ACETONE

METHANOL

WATER

20

ETHANOL

BUTYRALDEHYDE

METHYL ETHYL KETONE

25

n-PROPANOL

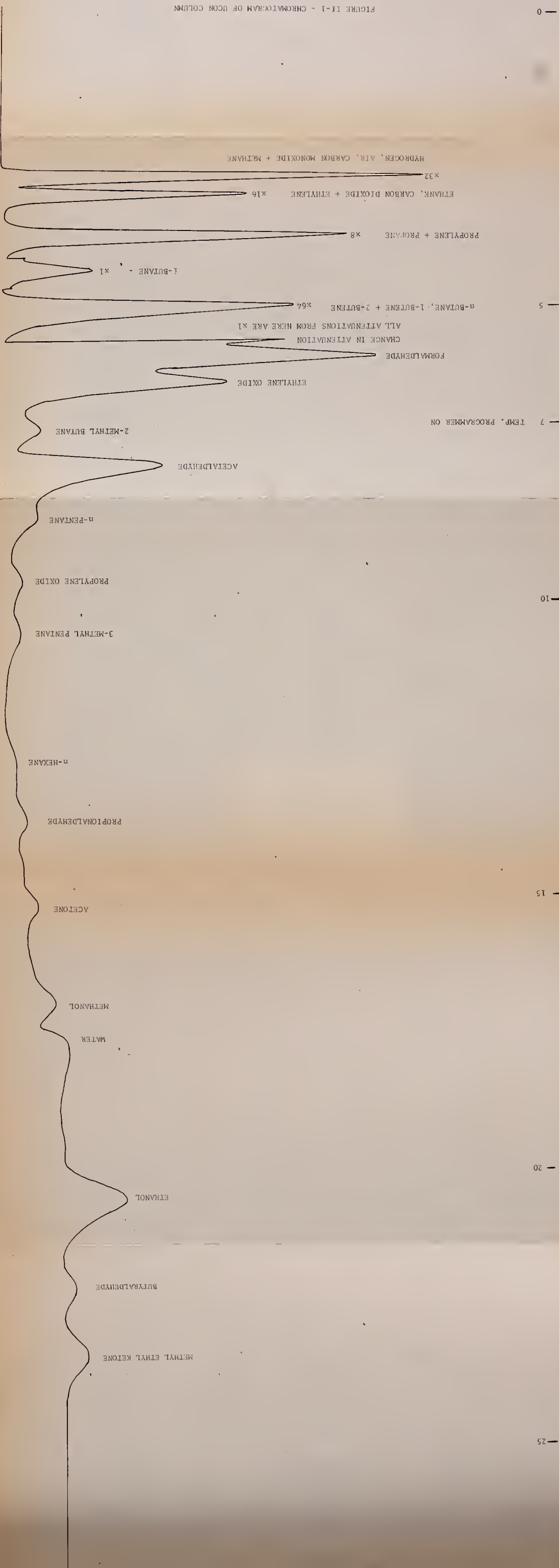
30

DIETHYL KETONE

35

0

FIGURE 11-1 - CHROMATOGRAM OF UCON COLUMN



5

7

10

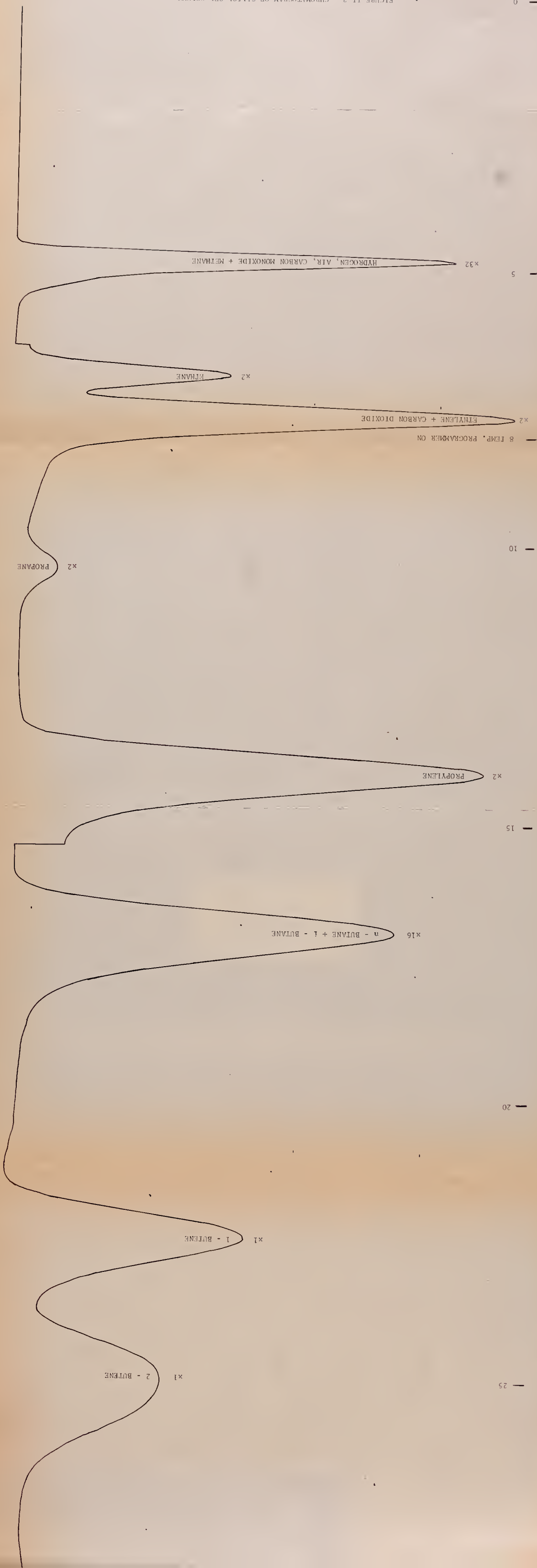
15

20

25









— 0  
TIME  
MINUTES

FIGURE II-3 - CHROMATOGRAM OF MOLYBDAN SILVE COLUMN



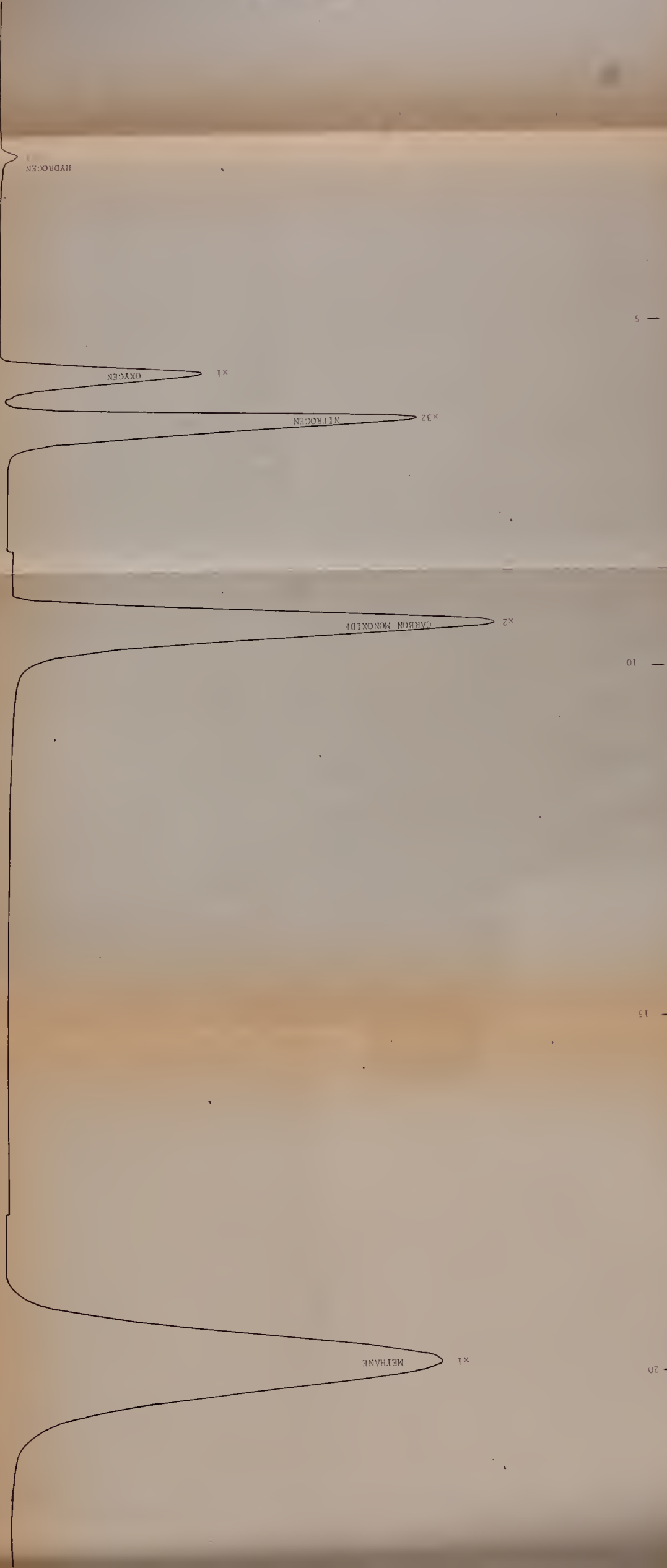
— 5

— 10



— 0  
TIME  
MINUTES

FIGURE 11-10 CHROMATOGRAM OF MOL. SIEVE - TITRICAL COLUMN







### APPENDIX III

#### CALIBRATION OF INSTRUMENTS



### A. Integral D/P Cells

The D/P Cell for the air was calibrated by passing a constant flow of air through it and measuring the air rate with a Natural Gas Meter made by the American Meter Company and certified accurate by the Standards Division of the Canadian Department of Trade and Commerce. The air flow rate, for each controller setting, was converted to standard conditions of 60°F and 1 atmosphere and then to a weight rate of flow. Orifice size and the range setting for the D/P cell are given in Table III-1 along with the experimental points used to determine the calibration curve. The calibration curve is shown as a log-log plot of the controller chart reading versus the weight rate of flow of the air in Figure III-1. The dotted line is the calibration curve supplied by Foxboro, the manufacturer of the D/P cell.

The D/P cell for the n-butane was calibrated with water and then converted to n-butane by the formula given by Foxboro as:

$$\text{Equivalent water flow (gpm)} = V G_b \sqrt{\frac{1}{G_f}}$$

where

- $V$  = flow of liquid n-butane in gpm at 60°F
- $G_b$  = specific gravity of n-butane at 60°F
- $G_f$  = specific gravity of n-butane at the flowing temperature





The rate of flow of water was measured at various controller settings by collecting the quantity of water flowing through the D/P cell in a certain length of time. The water rates were then converted to the rate of flow of n-butane at a flowing temperature of 75°F. Table III-2 gives a record of the orifice size and range setting for the D/P cell as well as the calibration points. The calibration curve, Figure III-2, is a log-log plot of the controller chart reading versus the n-butane flow rate in lb./hr. The dotted line is, once again, the calibration curve supplied by Foxboro for the orifice used.

#### B. Pressure Transmitter

The M/44 Pressure Transmitter was calibrated by using a 200 psig gauge that had been calibrated by a Dead Weight Tester and found to be accurate over the entire range. A nitrogen cylinder was fitted with a variable pressure regulator and connected to the transmitter and pressure gauge. Readings were taken at intervals of 20 psig up to 140 psig, the limit of the pressure regulator. The recorder was connected during the calibration and was found to record the transmitter pressure as a percentage of the range of the transmitter over the range calibrated. The points obtained are given in Table III-3.



### C. Thermocouples

All of the thermocouples were enclosed in a bundle and wrapped with asbestos tape. For calibration temperatures below  $350^{\circ}\text{C}$  a standard thermometer was included in the bundle to measure the correct temperature. For temperatures above  $350^{\circ}\text{C}$ , all thermocouple readings were compared to the reading of thermocouple number 6 which was chosen as the most accurate thermocouple on the basis of calibrations below  $350^{\circ}\text{C}$ . The bundle of thermocouples was inserted in an electric furnace and the furnace turned on. When the temperature in the furnace had stabilized at the desired temperature, readings of each thermocouple were taken along with readings of the standard thermometer or "standard" thermocouple. The desired temperature level was obtained by adjusting a rheostat connected to the heater. Care was taken during each reading to be sure that the temperature was not fluctuating. Any fluctuations could cause errors because different thermocouples required different times to reach equilibrium.

The thermocouples were checked at four temperatures levels, 330, 350, 400, and  $450^{\circ}\text{C}$  and were all found to be within  $\pm 3^{\circ}\text{F}$  of the true temperature. No calibration curves were plotted for the thermocouples as the errors were random. No corrections were made on the recorded temperatures and standard conversion tables were used to convert the thermocouple millivolt readings to temperatures.





Table III-1D/P Cell Calibration for Air

Orifice diameter	0.0595 inches
D/P Cell range	100 inches of water
Air temperature	73°F
Atmospheric pressure	28.09 inches of Hg

Controller Chart Reading %	Air Rate cu.ft./min.	Air Rate S.C.F.M.	Weight Rate of Flow lb/hr.
19.8	0.335	0.307	1.403
20.0	0.334	0.306	1.398
40.0	0.484	0.444	2.028
59.9	0.602	0.550	2.513
80.0	0.703	0.643	2.938
97.7	0.781	0.716	3.271

Table III-2D/P Cell Calibration for n-Butane

Orifice diameter	0.0200 inches
D/P Cell range	250 inches of water
Water temperature	72°F

Controller Chart Reading %	Water Rate U.S. GPM	Weight Rate of Flow of n-Butane lb./hr.
20.0	.0152	5.73
40.0	.0222	8.37
60.0	.0274	10.32
59.8	.0275	10.36
81.2	.0322	12.13
94.3	.0349	13.15
40.5	.0223	8.40
23.0	.0164	6.18





Table III-3Pressure Transmitter Calibration

Transmitter psig	Actual Pressure psig	Recorder Chart %
20	19.8	10.0
40	39.6	20.0
60	59.4	30.0
70	69.3	35.0
79	78.6	34.5
98	98.4	49.0
117	118.2	58.5
137	138.0	68.5



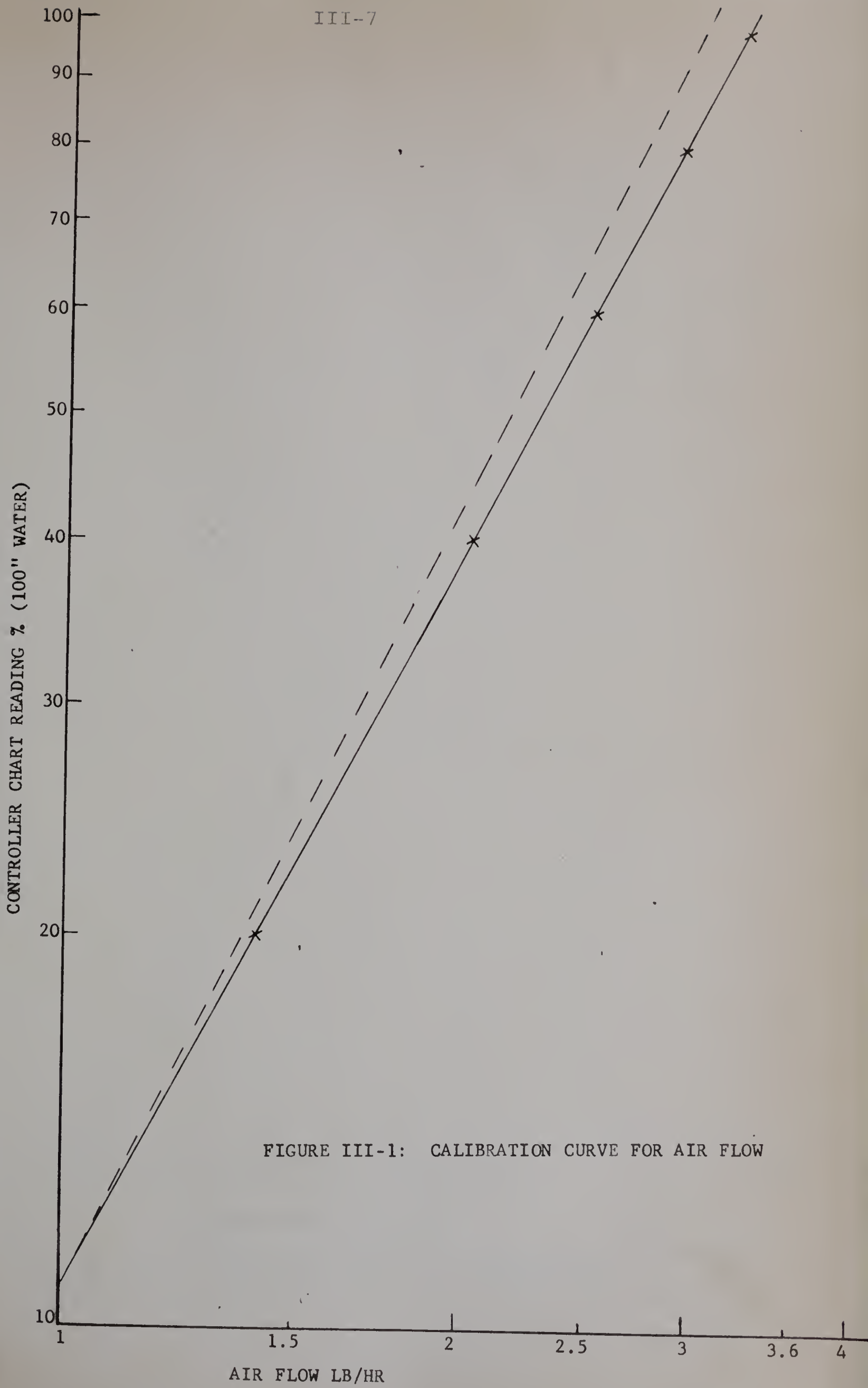


FIGURE III-1: CALIBRATION CURVE FOR AIR FLOW





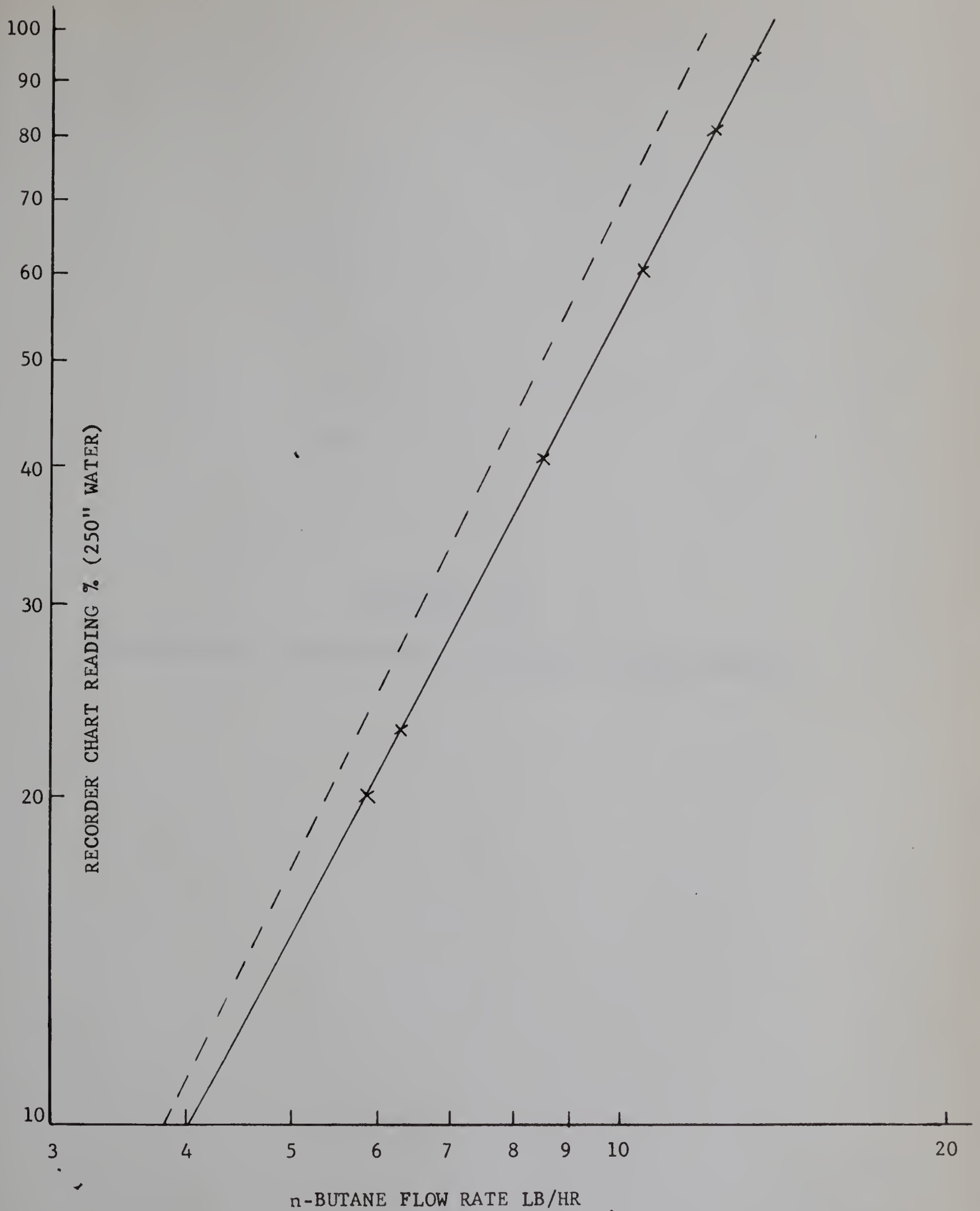


FIGURE III-2: CALIBRATION CURVE FOR n-BUTANE FLOW



#### APPENDIX IV

#### EXPERIMENTAL TEMPERATURES RECORDED IN THE REACTOR



The experimental temperatures, obtained for each run, are recorded in Table IV-1. All readings are the actual thermocouple recorded millivolts converted to degrees Fahrenheit. The readings have not been corrected for errors due to conduction and radiation between the thermocouple and reactor wall but the magnitude of the errors are calculated in Appendix V.

Temperatures that have an asterisk (\*) beside them are questionable and are not used. A reading for thermocouple 15 is not always reported as it was often below the range of the temperature recorder. The low temperature was caused by the position of the thermocouple at the reactor exit.





Table IV-1Experimental Temperature Profiles

Run Number	10	11	12	13	14	15	16	17	18
Thermo- couple Number	Temperature °F								
16	732	705	704	705	696	727	702	681	723
1	1129	679	679	680	665	782	688	729	785
2	1110	851	698	800	678	984	876	653	1095
3W	1003	*1027	*727	*1076	*705	917	*1113	637	1050
4	1073	1032	1023	1045	896	966	1102	656	1079
5	1047	1009	1036	1026	1040	946	1066	697	1047
6W	962	949	975	958	958	891	991		982
7	1021	988	1013	1000	1015	*885	1037	939	*947
8	989	964	989	975	983	912	1010	1058	1005
9W	913	906	934	913	909	859	939	980	944
10	967	947	973	*940	954	897	989	1023	987
11	946	932	959	940	941	885	968	994	970
12W	881	883	912	885	878	842	907	916	919
13	926	917	946	925	923	875	950	971	956
14	880	873	909	886	881	840	907	918	912
15W			684	659			680	674	710



## IV-4

Table IV-1 - continued

Run Number	19	20	21	22	23	24	25	26
Thermo- couple Number	Temperature °F							
16	685	702	687	723	700	792	909	699
1	762	691	667	733	671	764	876	682
2	919	912	802	1155	681	774	882	829
3W	*1216	*1207	*1246	1060	689	778	888	*1194
4	1161	1157	1206	1110	689	780	896	1164
5	1116	1113	1126	1080	697	789	904	1103
6W	1047	1035	1045	997	708	801	910	1023
7	*987	1086	1096	1053	707	799	908	1071
8	1071	1059	1067	1026	714	805	924	1046
9W	1007	990	997	953	722	804	927	976
10	1052	1037	1045	1002	724	809	937	1026
11	1034	1021	1026	983	728	816	946	1006
12W	980	959	963	915	742	827	952	945
13	1019	1002	1008	961	739	827	955	989
14	971	955	963	918	730	815	936	948
15W	746	709	701	667				714





The first effect of the new method is that the temperature of the liquid is now measured at the point of the thermometer bulb, instead of at the top of the liquid column. This is a very important improvement, because the temperature of the liquid at the top of the column is usually higher than at the bottom, due to the heat of the bulb. The second effect is that the temperature of the liquid is now measured at the point of the thermometer bulb, instead of at the top of the liquid column. This is a very important improvement, because the temperature of the liquid at the top of the column is usually higher than at the bottom, due to the heat of the bulb.

The third effect of the new method is that the temperature of the liquid is now measured at the point of the thermometer bulb, instead of at the top of the liquid column. This is a very important improvement, because the temperature of the liquid at the top of the column is usually higher than at the bottom, due to the heat of the bulb. The fourth effect is that the temperature of the liquid is now measured at the point of the thermometer bulb, instead of at the top of the liquid column. This is a very important improvement, because the temperature of the liquid at the top of the column is usually higher than at the bottom, due to the heat of the bulb.

APPENDIX V  
THERMOCOUPLE CORRECTIONS



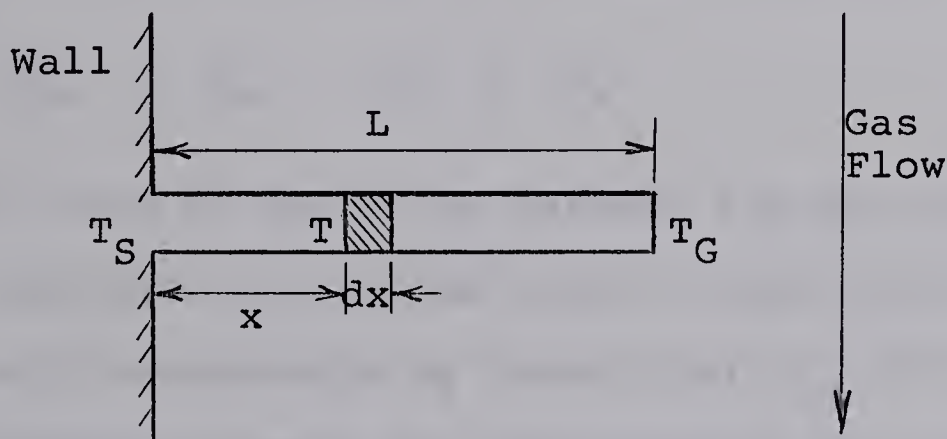
The thermocouple is a device which produces an electric current when two different metals are joined together and the junctions are kept at different temperatures. The current is produced by the Seebeck effect. The thermocouple is used to measure temperature differences. The thermocouple is a very sensitive device and can be used to measure temperature differences as small as 0.01°C. The thermocouple is a very important device in many scientific and industrial applications. The thermocouple is a very important device in many scientific and industrial applications. The thermocouple is a very important device in many scientific and industrial applications.



Eleven thermocouples were installed in the gas stream normal to the gas flow to measure the temperature in the gas phase. The thermocouples were inserted through the reactor wall with the tips at the center of the reactor. Errors were expected in the thermocouple readings because the surface area of the thermocouples in contact with the gas stream was small and because the thermocouples were attached to the reactor wall.

No attempt was made to correct all of the thermocouple readings for each experimental run but the following calculations serve to indicate the magnitude of the errors.

Consider a heat balance around a small element of the thermocouple illustrated in the diagram:



$T$  = the temperature of the thermocouple at a distance  $x$  from the reactor wall  $^{\circ}\text{R}$

$T_S$  = reactor wall temperature  $^{\circ}\text{R}$

$T_g$  = true gas temperature  $^{\circ}\text{R}$

$T_p$  = temperature at the tip of the thermocouple

$b$  = perimeter of the thermocouple =  $1.638 \times 10^{-2}$  ft.

$S$  = cross-sectional area of the thermocouple (metal only) =  $1.153 \times 10^{-5}$  ft.<sup>2</sup>



$D_o$  = outside diameter of thermocouple =  $5.22 \times 10^{-3}$  ft.

$D_i$  = inside diameter of thermocouple =  $3.54 \times 10^{-3}$  ft.

$L$  = length of thermocouple =  $2.60 \times 10^{-2}$  ft.

$h_c$  = convective heat transfer coefficient  
BTU/hr.ft.<sup>2</sup> °F

$h_r$  = radiant heat transfer coefficient, BTU/hr.ft.<sup>2</sup> °F

$k$  = thermal conductivity of thermocouple = 12.1  
BTU/hr.ft.<sup>2</sup> °F/ft.

$\epsilon$  = emissivity of the thermocouple

$G$  = mass flow rate of gas, lb/ft.<sup>2</sup>hr.

$k_f$  = thermal conductivity of gas = .0307 BTU/hr.ft.<sup>2</sup>  
°F/ft.

$\mu_f$  = viscosity of gas = 0.0586 lb/ft.hr.

$$Q_{gr} + Q_c = Q_r + Q_k \quad (V-1)$$

where  $Q_{gr}$  is the rate of heat flow between the gas and thermocouple by gas radiation,  $Q_c$  is the rate of heat transfer between the gas and thermocouple by convection,  $Q_r$  is the radiant heat exchange between the thermocouple and the reactor wall, and  $Q_k$  is the heat transferred by conduction from the thermocouple to the reactor wall. By neglecting gas radiation, thermal gradients in the thermocouple wall, and the effect of the tip of the thermocouple, the heat balance, in differential form, becomes:

$$h_c b \, dx \, (T_g - T) = 1.713 \times 10^{-9} \, \epsilon b \, dx \, (T^4 - T_s^4) - ks \left( \frac{d^2 T}{dx^2} \right) dx \quad (V-2)$$





The absolute temperature to the fourth power may be removed from equation (V-2) by using a radiant heat transfer coefficient defined by the equation:

$$\begin{aligned} Q_R &= h_r b \, dx \, (T - T_s) \\ &= 1.713 \times 10^{-9} \, \epsilon b \, dx \, (T^4 - T_s^4) \end{aligned} \quad (V-3)$$

$$h_r = 1.713 \times 10^{-9} \, \epsilon \frac{(T^4 - T_s^4)}{(T - T_s)} \quad (V-4)$$

Substituting equation (V-3) into equation (V-2) gives

$$h_c b \, dx \, (T_g - T) = h_r b \, dx \, (T - T_s) - kS \left( \frac{d^2 T}{dx^2} \right) dx \quad (V-5)$$

Rearranging equation (V-5) produces the differential equation

$$-\frac{d^2 T}{dx^2} = \frac{h_c b}{kS} (T_g - T) - \frac{h_r b}{kS} (T - T_s) \quad (V-6)$$

The integration of equation (V-6) is difficult unless certain simplifying assumptions are made. The radiant heat transfer coefficient is a function of the thermocouple and wall temperatures, but an average value may be used without causing too great an error, providing that the coefficient is not too large. The convective heat transfer coefficient is a function of the fluid properties and may be assumed constant. For a thermocouple of constant cross section the perimeter and cross-section are constant. The flowing gas temperature and the wall temperature are constant for any point in the reactor.



Rearranging equation (V-6) gives

$$-\frac{d^2 T}{dx^2} + \frac{(h_c + h_r)b}{kS} (T - T_g) = -\frac{h_r b}{kS} (T_g - T_s) \quad (V-7)$$

or

$$\frac{d^2 (T - T_g)}{dx^2} - a^2 (T - T_g) = \emptyset \quad (V-8)$$

where

$$a^2 = \frac{(h_c + h_r)b}{kS}$$

and

$$\emptyset = \frac{h_r b}{kS} (T_g - T_s)$$

Boundary conditions that apply for the solution of equation (V-8) are:

$$(1) \quad (T - T_g)_{x=0} = T_s - T_g$$

$$(2) \quad \left. \frac{d(T - T_g)}{dx} \right|_{x=L} = 0$$

The general solution of equation (V-8) is

$$T - T_g = A \cosh ax + B \sinh ax - \frac{\emptyset}{a^2} \quad (V-9)$$

where A and B are constants

A and B are evaluated by substituting the two boundary conditions into equation (V-9) to give the solution for the thermocouple temperature at any point as:





$$\frac{T_g - T}{T_g - T_s} = \left( \frac{h_c}{h_c + h_r} \right) \frac{\cosh a (L - x)}{\cosh aL} + \left( \frac{h_r}{h_c + h_r} \right) \quad (V-10)$$

At the thermocouple tip,  $x = L$  and  $T = T_p$ , and the thermocouple correction is given by:

$$\begin{aligned} \frac{T_g - T_p}{T_g - T_s} = & \left( \frac{h_c}{h_c + h_r} \right) \left( \cosh \sqrt{\frac{(h_c + h_r)b}{kS}} L \right)^{-1} \\ & + \left( \frac{h_r}{h_c + h_r} \right) \end{aligned} \quad (V-11)$$

Sample calculations to determine the magnitude of the thermocouple correction are made for the following temperature and flow conditions which are representative of the experimental temperatures:

$$T_s = 820^{\circ}\text{F} = 1280^{\circ}\text{R}$$

$$T_p = 900^{\circ}\text{F} = 1360^{\circ}\text{R}$$

$$\text{Flow Rate} = 12 \text{ lb./hr.}$$

$$\text{Composition} = 60 \text{ mole \% n-butane and } 40 \text{ mole \% air}$$

The convection heat transfer coefficient is given by the equation

$$\frac{h_c D_o}{k_f} = 0.615 \left( \frac{D_o G}{\mu_f} \right)^{0.466} \quad (V-12)$$

By substituting the values of the fluid properties, flow rate, and thermocouple size into equation (V-12),  $h_c$  is calculated as  $65.6 \text{ BTU/hr.ft.}^2 \text{ }^{\circ}\text{F}$ .



The radiant heat transfer coefficient is given by equation (V-4).

At the thermocouple tip,

$$h_r = 1.713 \times 10^{-9} \epsilon \left( \frac{T_p^4 - T_s^4}{T_p - T_s} \right)$$

At the base of the thermocouple,  $h_r = 0$  as  $T = T_s$ .

For a thermocouple of emissivity equal to 0.5, the radiant heat transfer coefficient at the tip is 7.8 BTU/hr.ft<sup>2</sup> °F. Thus, the average radiant heat transfer coefficient is 3.9 BTU/hr.ft<sup>2</sup> °F.

To allow for the bare tip of the thermocouple, McAdams(22) recommends increasing the length of the thermocouple by an amount  $D_o/4$ .

Substituting all values into equation (V-11) gives

$$\frac{T_g - T_p}{T_g - T_s} = 0.131 \quad (V-13)$$

Solving equation (V-13) gives  $T_g = 912^\circ\text{F}$ .

Thus, the thermocouple correction is 12°F as the gas temperature is 912°F and the thermocouple reads 900°F. This is representative of the experimental temperature conditions because, in most cases, there is only about a 60°F difference between the wall and thermocouple temperatures. At higher temperatures the radiant heat transfer coefficient becomes more important but the correction is still accurate because of increased convective heat transfer coefficient.



The first step in the calculation of the results is the determination of the total number of observations. This is done by adding the number of observations for each of the different categories of the independent variable. The second step is the calculation of the mean for each category. This is done by dividing the sum of the observations for each category by the number of observations in that category. The third step is the calculation of the standard deviation for each category. This is done by taking the square root of the variance for each category. The fourth step is the calculation of the correlation coefficient. This is done by dividing the covariance of the two variables by the product of their standard deviations. The fifth step is the calculation of the coefficient of determination. This is done by squaring the correlation coefficient. The sixth step is the calculation of the F-ratio. This is done by dividing the mean square for the treatment by the mean square for the error. The seventh step is the calculation of the p-value. This is done by looking up the F-ratio in the F-distribution table. The eighth step is the calculation of the confidence interval. This is done by adding and subtracting the standard error of the mean from the mean. The ninth step is the calculation of the power of the test. This is done by looking up the power of the test in the power table. The tenth step is the calculation of the effect size. This is done by dividing the mean square for the treatment by the total mean square.

## APPENDIX VI

### METHOD OF CALCULATION OF RESULTS





$m$  = average molecular weight of feed stream.

$P$  = reactor pressure, psia.

$R$  = gas constant.

$T$  = absolute temperature of reaction gases at the entrance,  $^{\circ}\text{R}$ .

$u_o$  = velocity of gas at entrance to reactor, ft./sec.

$w$  = weight rate of flow of feed stream, lb./hr.

$\rho$  = density of reaction gases at the entrance, lb./ft.<sup>3</sup>

$\tau_o$  = residence time of the gases in the reactor based on entrance conditions, sec.

$\mu$  = viscosity of gases at the entrance, lb./ft.hr.

For each product sample, calculations are carried out for mole per cent of each component, moles per mole of nitrogen, moles formed per mole of oxygen reacted, and moles formed per mole of n-butane reacted. Carbon, hydrogen, and oxygen balances are determined for each sample along with per cent oxygen and n-butane reacted. Detailed calculations are given below.

Calculate  $\frac{\text{Component Area}}{\text{Relative Response Factor}}$  for each com-

ponent or group of components on the Ucon column and find the total

$$TOT_{UC} = \sum \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Subscript UC refers to the Ucon column.



$$\% \text{ Component}_{\text{UC}} = \frac{100}{\text{TOT}_{\text{UC}}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Peaks 1, 2, 3, and 5 on the chromatogram of the Ucon column, Figure II-1, are for groups of components and the other three chromatograph columns are used to separate these groups into individual components. Repeat the above calculations for each of the other three columns.

$$\% \text{ Component}_{\text{SiO}_2} = \frac{100}{\text{TOT}_{\text{SiO}_2}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Subscript  $\text{SiO}_2$  refers to the Silica Gel Column.

$$\% \text{ Component}_{\text{MS}} = \frac{100}{\text{TOT}_{\text{MS}}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Subscript MS refers to the Molecular Sieve Column.

$$\% \text{ Component}_{\text{MS-C}} = \frac{100}{\text{TOT}_{\text{MS-C}}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Subscript MS-C refers to the Molecular Sieve-Charcoal Column.

Calculate percentages of ethane, ethylene, and carbon dioxide on the Silica Gel Column by combining the results of the Molecular Sieve and Silica Gel Columns as outlined.

$$\% \text{ Ethane} = \% \text{ Ethane on Silica Gel Column}$$

$$\% \text{ Ethylene} = \% \text{ Ethane on Silica Gel} \times \frac{\% \text{ Ethylene on Mol. Sieve}}{\% \text{ Ethane on Mol. Sieve}}$$

$$\% \text{ Carbon Dioxide} = \% (\text{Ethylene} + \text{Carbon Dioxide}) \text{ on Silica Gel} - \% \text{ Ethylene}$$





$$\% C_2's = \% \text{ Ethane} + \% \text{ Ethylene} + \% \text{ Carbon Dioxide on Silica Gel Column}$$

The percentages of the individual components are related to the appropriate peak on the Ucon column to give the overall composition of the product analysis.

Peak 1 on the Ucon column is a combination of hydrogen, oxygen, nitrogen, carbon monoxide, and methane and the components are separated on the Molecular Sieve-Charcoal column. The overall composition for each component of peak 1 is given by

$$\text{Overall \% Component} = \% \text{ Component}_{\text{MS-C}} \times \text{mole fraction of peak 1 on Ucon column}$$

Peak 2 on the Ucon column is ethane, carbon dioxide, and ethylene and the overall composition is given by:

$$\text{Overall \% Ethane} = \frac{\% \text{ Ethane on Silica Gel Column}}{\% C_2's} \times \text{mole fraction of peak 2 on Ucon Column.}$$

Similar equations apply for ethylene and carbon dioxide.

Peak 3 on the Ucon column represents propane and propylene and the overall compositions are calculated by the following equations

$$\text{Overall \% Propylene} = \frac{\% \text{ Propylene on Silica Gel Column}}{\% C_3's} \times \text{mole fraction of peak 3 on the Ucon column}$$



where

$$\% C_3's = \% \text{ Propane} + \% \text{ Propylene on the Silica Gel Column.}$$

A similar equation may be written for propane n-Butane, 1-butene, and 2-butene are combined in peak 5 on the Ucon column and may be separated and the overall composition calculated by equations of the type

$$\text{Overall \% n-Butane} = \frac{\% \text{ n-Butane on Silica Gel Column}}{\% C_4's} \times \text{mole fraction of peak 5 on the Ucon column.}$$

where

$$\% C_4's = \% \text{ n-Butane} + \% \text{ 1-Butene} + \% \text{ 2-Butene on the Silica Gel Column.}$$

The total analysis has now been calculated for the 32 components listed in Table VII-1.

The following calculations are made to determine carbon, hydrogen, and oxygen balances and percent oxygen and n-butane reacted.

$$\frac{\text{Moles component}}{\text{Mole Nitrogen}} = \frac{\text{Mole \% component}}{\text{Mole \% Nitrogen}}$$

$$\text{Carbon Balance} = \frac{\text{Moles component}}{\text{Mole Nitrogen}} \times \text{Number of carbon atoms in component}$$



$$\text{Hydrogen Balance} = \frac{\text{Moles component}}{\text{Mole Nitrogen}} \times \text{Number of hydrogen atoms in component}$$

$$\text{Oxygen Balance} = \frac{\text{Moles component}}{\text{Mole Nitrogen}} \times \text{Number of oxygen atoms in component}$$

$$\% \text{ Carbon Balance} = \frac{100 \times \text{total Carbon Balance}}{4 \times \frac{\text{moles n-Butane}}{\text{Mole Nitrogen}} \text{ in the feed}}$$

Similar equations apply for the % Hydrogen Balance and % Oxygen Balance.

$$\% \text{ Oxygen Reacted} = 100 \left( \frac{\frac{\text{mole Oxygen}}{\text{mole Nitrogen}} \text{ in the feed} - \frac{\text{Moles Oxygen}}{\text{mole Nitrogen}}}{\frac{\text{moles Oxygen}}{\text{mole Nitrogen}} \text{ in the feed}} \right)$$

$$\% \text{ n-Butane Reacted} =$$

$$100 \left( \frac{\frac{\text{moles n-Butane}}{\text{mole Nitrogen}} \text{ in the feed} - \frac{\text{moles n-Butane}}{\text{mole Nitrogen}}}{\frac{\text{moles n-Butane}}{\text{mole Nitrogen}} \text{ in the feed}} \right)$$

The final calculations are made to determine the moles of each component formed per mole of oxygen and n-butane reacted.

$$\frac{\text{Moles component formed}}{\text{Mole Oxygen Reacted}} = \frac{\frac{\text{moles component formed}}{\text{mole Nitrogen}}}{\frac{\text{moles Oxygen Reacted}}{\text{mole Nitrogen}}}$$





$$\frac{\text{Moles component formed}}{\text{Mole n-Butane Reacted}} = \frac{\frac{\text{moles component formed}}{\text{mole Nitrogen}}}{\frac{\text{moles n-Butane Reacted}}{\text{mole Nitrogen}}}$$

The computer program that was used in the calculation of all the results described here and presented in Appendix VII follows.



## PRODUCT COMPOSITION

## FORTRAN SOURCE LIST

ISN SOURCE STATEMENT

```

0 $IBFTC PRCOMP NOLIST,NODECK
1   DIMENSION UCMR(23),SCMR(5),SMMR(2),SIMR(7),ARB(32),HYD(32),
   1XYO(32),UCAR(23),SCAR(5),SMAR(2),SIAR(7),UC(23),UCON(23),SC(5),
   2S13XC(5),SH(2),S175(2),SI(7),SIC(7),SIC2(3),SIO2(9),PCNT(32),
   3PMN2(32),ARBM(32),HYDM(32),XYOM(32),PMOR(32),PMCR(32)
2   READ (5,3) (UCMR(I),I=1,23),(SCMR(I),I=1,5),(SMMR(I),I=1,2),
   1   (SIMR(I),I=1,7)
23  3 FORMAT(1X,10F6.3/1X,10F6.3/1X,3F6.3/1X,5F6.3/1X,2F6.3/1X,7F6.3)
24  READ (5,25) (ARB(I),I=1,32),(HYD(I),I=1,32),(XYO(I),I=1,32)
41  25 FORMAT(1X,16F4.1/1X,16F4.1/1X,14F5.1/1X,14F5.1/1X,4F5.1/
   1   1X,16F4.1/1X,16F4.1)
C** INITIAL CONDITIONS
42  NUM = 1
43  DO 70 K=1,14
44  NUM = NUM+1
45  READ (5,1) AIR,BUT,TEMP,M,PRS
47  1 FORMAT(1X,2F6.2,F8.2,I3,F6.2)
50  TOTW = AIR + BUT
51  AIRM = AIR/28.855
52  BUTM = BUT/58.124
53  TOT = AIRM + BUTM
54  PCAIR = 100.0*AIRM/TOT
55  PCO2 = 0.21*PCAIR
56  PCN2 = 0.79*PCAIR
57  PCC4 = 100.0*BUTM/TOT
60  RON = PCO2/PCN2
61  RNN = PCN2/PCN2
62  RC4N = PCC4/PCN2
63  XAIR = 0.01*PCAIR
64  XCC4 = 0.01*PCC4
65  AVMW = 28.855*XAIR + 58.124*XCC4
66  DNS = AVMW*PRS/(10.731*(460.0 + TEMP))
67  VEL = TOTW/(7.670*DNS)
70  TIME = 9.75/VEL
71  VAIR = 2.42*(0.0175 + 0.000019*TEMP)
72  VBUT = 2.42*(0.0063 + 0.0000134*TEMP)
73  VISC = (5.372*XAIR*VAIR+7.624*XCC4*VBUT)/(5.372*XAIR+7.624*XCC4)
74  REN = 187.5*VEL*DNS/VISC
75  IREN = REN
76  WRITE (6,40) NUM,M
77  40 FORMAT(1H1/1H2,44X,5HVII -,I3/////21X,9HRUN NO = ,I3)
100  WRITE (6,41)
101  41 FORMAT(1HJ,20X,27HREACTOR ENTRANCE CONDITIONS )
102  WRITE (6,2) AIR,BUT,TEMP,PRS,PCO2,PCN2,PCC4,RON,RNN,RC4N,DNS,VEL,
   1TIME,IREN
103  2 FORMAT(1HJ,20X,6HAIR = ,F6.2,6H LB/HR,10X,9HBUTANE = ,F6.2,6H LB/H
   1R//21X,14HTEMPERATURE = ,F8.2,7H DEG F ,//21X,11HPRESSURE = ,F6.2,
   29H LB/SQ IN,//21X,9HOXYGEN = ,F9.4,12H NITROGEN = ,F9.4,10H BUTANE
   3 = ,F9.4,9H MOL PCNT//21X,9HOXY/N = ,F9.4,12H NIT/N = ,F9.4,
   410H BUT/N = ,F9.4,9H MOLS/MN2//21X,25HDENSITY OF GAS MIXTURE = ,
   5F8.4,9H LB/CU FT //21X,15HGAS VELOCITY = ,F6.2,7H FT/SEC //21X,
   648HRESIDENCE TIME BASED ON ENTRANCE CONDITIONS = ,F6.2,4H SEC //
   721X,18HREYNOLDS NUMBER = ,I8)
104  100 READ (5,4) N
106  NUM = NUM+1

```







ISN SOURCE STATEMENT

```
107      4 FORMAT(1X,I2)
110      READ (5,5) (UCAR(I),I=1,23),(SCAR(I),I=1,5),(SMAR(I),I=1,2),
111      1 (SIAR(I),I=1,7)
131      5 FORMAT(1X,8F8.3/1X,8F8.3/1X,7F8.3/1X,5F8.3/1X,2F8.3/1X,7F8.3)
C**      CALCULATIONS ON UCON COLUMN
132      SUC = 0.0
133      DO 10 I=1,23
134      UC(I) = UCAR(I)/UCMR(I)
135      10 SUC = SUC+UC(I)
137      DO 11 I=1,23
140      11 UCON(I) = 100.0*UC(I)/SUC
C**      CALCULATIONS ON MOLECULAR SEIVE TYPE 13X + CHARCOAL COLUMN
142      SSC = 0.0
143      DO 12 I=1,5
144      SC(I) = SCAR(I)/SCMR(I)
145      12 SSC = SSC+SC(I)
147      DO 13 I=1,5
150      13 S13XC(I) = (SC(I)/SSC)*UCON(1)
C**      CALCULATIONS ON MOLECULAR SEIVE COLUMN AT 175 DEG C
152      SSH = 0.0
153      DO 14 I=1,2
154      SH(I) = SMAR(I)/SMMR(I)
155      14 SSH = SSH+SH(I)
157      DO 15 I=1,2
160      15 S175(I) = SH(I)/SSH
C**      CALCULATIONS ON SILICA GEL COLUMN
162      SSI = 0.0
163      DO 16 I=1,7
164      SI(I) = SIAR(I)/SIMR(I)
165      16 SSI = SSI+SI(I)
167      DO 17 I=1,7
170      17 SIC(I) = SI(I)/SSI
172      SIC2(1) = SIC(1)
173      SIC2(3) = SIC(1)*S175(2)/S175(1)
174      SIC2(2) = SIC(2)-SIC2(3)
175      SC2 = SIC2(1)+SIC2(2)+SIC2(3)
176      SC3 = SIC(3)+SIC(4)
177      SC4 = SIC(5)+SIC(6)+SIC(7)
200      DO 18 I=1,9
201      IF (I.LE.3) GOTO 19
204      IF (I.LE.5) GO TO 20
207      IF (I.EQ.6) GO TO 21
212      SIO2(I) = (SIC(I-2)/SC4)*UCON(5)
213      GO TO 18
214      19 SIO2(I) = (SIC2(I)/SC2)*UCON(2)
215      GO TO 18
216      20 SIO2(I) = (SIC(I-1)/SC3)*UCON(3)
217      GO TO 18
220      21 SIO2(I) = UCON(4)
221      18 CONTINUE
C**      PRODUCT ANALYSIS MOL PERCENT
223      SPCNT = 0.0
224      DO 22 I=1,32
225      IF (I.LE.5) GO TO 23
230      IF (I.LE.14) GO TO 24
```



ISN SOURCE STATEMENT

```

233      PCNT(I) = UCON(I-9)
234      GO TO 22
235      23 PCNT(I) = S13XC(I)
236      GO TO 22
237      24 PCNT(I) = SIO2(I-5)
240      22 SPCNT = SPCNT+PCNT(I)
C**      CARBON HYDROGEN OXYGEN BALANCES
242      SPMN2 = 0.0
243      SARBM = 0.0
244      SHYDM = 0.0
245      SXYOM = 0.0
246      DO 26 I=1,32
247      PMN2(I) = PCNT(I)/PCNT(3)
250      ARBM(I) = PMN2(I)*ARB(I)
251      HYDM(I) = PMN2(I)*HYD(I)
252      XYOM(I) = PMN2(I)*XYO(I)
253      SPMN2 = SPMN2+PMN2(I)
254      SARBM = SARBM+ARBM(I)
255      SHYDM = SHYDM+HYDM(I)
256      26 SXYOM = SXYOM+XYOM(I)
260      XYOR = RON-PMN2(2)
261      BUTR = RC4N-PMN2(12)
262      PCOR = 100.0*XYOR/RON
263      PCBR = 100.0*BUTR/RC4N
264      PCARB = 100.0*SARBM/(4.0*RC4N)
265      PCHYD = 100.0*SHYDM/(10.0*RC4N)
266      PCXYO = 100.0*SXYOM/(2.0*RON)
C**      PRODUCT SELECTIVITIES
267      DO 27 I=1,32
270      PMOR(I) = PMN2(I)/XYOR
271      27 PMCR(I) = PMN2(I)/BUTR
273      WRITE (6,29) NUM,M,N
274      29 FORMAT(1H2,44X,5HVII -,I3/////21X,9HRUN NO = ,I3,2X,12HSAMPLE NO =
1 ,I2)
275      30 WRITE(6,31)
276      31 FORMAT(1HJ,21X,60HPROD NO MOL PERCENT MOLS/MOL N2 MOLS/MOXY R
1MOLS/MBUT R )
277      DO 60 I=1,32
300      32 FORMAT(1H ,22X,I3,2X,4(2X,F11.6))
301      60 WRITE(6,32)I,PCNT(I),PMN2(I),PMOR(I),PMCR(I)
303      WRITE(6,33)SPCNT,SPMN2,SARBM,PCARB,SHYDM,PCHYD,SXYOM,PCXYO,
1PCOR,PCBR
304      33 FORMAT(1HJ,21X,6HTOTALS,2(2X,F11.6)//21X,17HCARBON BALANCE ,
1F11.6,13H LB AT/MOLN2.,F8.2,8H PERCENT/21X,17HHYDROGEN BALANCE ,
2F11.6,13H LB AT/MOLN2.,F8.2,8H PERCENT/21X,17HOXYGEN BALANCE ,
3F11.6,13H LB AT/MOLN2.,F8.2,8H PERCENT//21X,17HPERCENT O2 REACT ,
4F10.4,4X,17HPERCENT C4 REACT ,F10.4)
305      IF (N.LE.4) GO TO 100
310      70 CONTINUE
312      CONTINUE
313      END

```





APPENDIX VII  
EXPERIMENTAL RESULTS





RUN NO = 10

REACTOR ENTRANCE CONDITIONS

AIR = 2.40 LB/HR BUTANE = 7.14 LB/HR

TEMPERATURE = 732.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.4783 NITROGEN = 31.8946 BUTANE = 59.6270 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.8695 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.1937 LB/CU FT

GAS VELOCITY = 6.42 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.52 SEC

REYNOLDS NUMBER = 4578



## VII - 3

RUN NO = 10 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.732696	0.024938	0.101565	0.045354
2	0.596172	0.020291	0.082641	0.036904
3	29.381210	1.000000	4.072791	1.818721
4	2.925015	0.099554	0.405462	0.181061
5	3.083264	0.104940	0.427399	0.190857
6	1.850644	0.062987	0.256534	0.114556
7	1.843272	0.062736	0.255512	0.114100
8	5.510522	0.187553	0.763863	0.341106
9	0.429137	0.014606	0.059487	0.026564
10	6.694667	0.227855	0.928008	0.414406
11	0.149057	0.005073	0.020662	0.009227
12	38.773300	1.319663	5.374713	2.400100
13	1.396482	0.047530	0.193579	0.086443
14	1.100343	0.037451	0.152528	0.068112
15	1.049117	0.035707	0.145428	0.064941
16	0.543126	0.018485	0.075288	0.033620
17	0.079620	0.002710	0.011037	0.004929
18	1.086613	0.036983	0.150625	0.067262
19	0.098265	0.003344	0.013621	0.006083
20	0.083336	0.002836	0.011552	0.005159
21	0.000000	0.000000	0.000000	0.000000
22	0.036135	0.001230	0.005009	0.002237
23	0.107147	0.003647	0.014853	0.006632
24	0.000000	0.000000	0.000000	0.000000
25	0.104862	0.003569	0.014536	0.006491
26	1.526094	0.051941	0.211545	0.094466
27	0.526915	0.017934	0.073040	0.032617
28	0.116176	0.003954	0.016104	0.007191
29	0.093946	0.003197	0.013023	0.005815
30	0.082874	0.002821	0.011488	0.005130
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999997	3.403536		

CARBON	BALANCE	7.414810 LB AT/MOLN2.	99.15 PERCENT
HYDROGEN	BALANCE	17.736551 LB AT/MOLN2.	94.87 PERCENT
OXYGEN	BALANCE	0.446684 LB AT/MOLN2.	84.02 PERCENT

PERCENT O2 REACT	92.3667	PERCENT C4 REACT	29.4109
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RUN NO = 10 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.843212	0.028931	0.114723	0.044943
2	0.397600	0.013642	0.054096	0.021192
3	29.145543	1.000000	3.965407	1.553454
4	3.567761	0.122412	0.485413	0.190161
5	3.531474	0.121167	0.480476	0.188227
6	2.164134	0.074253	0.294442	0.115348
7	1.948591	0.066857	0.265116	0.103860
8	5.749314	0.197262	0.782225	0.306438
9	0.541823	0.018590	0.073718	0.028879
10	7.231826	0.248128	0.983929	0.385455
11	0.136669	0.004689	0.018595	0.007284
12	35.725823	1.225773	4.860689	1.904182
13	1.581162	0.054251	0.215126	0.084276
14	1.242645	0.042636	0.169068	0.066233
15	0.976736	0.033512	0.132890	0.052060
16	0.654283	0.022449	0.089019	0.034873
17	0.084318	0.002893	0.011472	0.004494
18	1.087391	0.037309	0.147945	0.057958
19	0.105131	0.003607	0.014304	0.005603
20	0.096659	0.003316	0.013151	0.005152
21	0.000000	0.000000	0.000000	0.000000
22	0.050568	0.001735	0.006880	0.002695
23	0.082651	0.002836	0.011245	0.004405
24	0.056034	0.001923	0.007624	0.002987
25	0.164028	0.005628	0.022317	0.008743
26	1.857980	0.063748	0.252788	0.099030
27	0.615599	0.021122	0.083756	0.032811
28	0.105978	0.003636	0.014419	0.005649
29	0.108638	0.003727	0.014781	0.005790
30	0.100592	0.003451	0.013686	0.005362
31	0.045846	0.001573	0.006238	0.002444
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999998	3.431056
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CARBON	BALANCE	7.278722 LB AT/MOLN2.	97.34 PERCENT
HYDROGEN	BALANCE	17.330080 LB AT/MOLN2.	92.70 PERCENT
OXYGEN	BALANCE	0.487641 LB AT/MOLN2.	91.72 PERCENT

PERCENT O2 REACT	94.8681	PERCENT C4 REACT	34.4331
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## VII - 5

RUN NO = 10 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.909013	0.031438	0.124370	0.052641
2	0.377101	0.013042	0.051594	0.021838
3	28.914184	1.000000	3.955998	1.674431
4	3.342482	0.115600	0.457314	0.193564
5	3.551983	0.122846	0.485977	0.205697
6	2.261954	0.078230	0.309477	0.130991
7	1.982184	0.068554	0.271200	0.114789
8	5.768368	0.199500	0.789220	0.334048
9	0.562082	0.019440	0.076903	0.032550
10	6.709097	0.232035	0.917929	0.388526
11	0.153742	0.005317	0.021035	0.008903
12	36.787001	1.272282	5.033146	2.130349
13	1.568994	0.054264	0.214668	0.090861
14	1.297309	0.044868	0.177496	0.075128
15	0.773231	0.026742	0.105792	0.044778
16	0.597976	0.020681	0.081814	0.034629
17	0.068890	0.002383	0.009425	0.003989
18	1.152410	0.039856	0.157671	0.066737
19	0.083160	0.002876	0.011378	0.004816
20	0.086543	0.002993	0.011841	0.005012
21	0.000000	0.000000	0.000000	0.000000
22	0.058809	0.002034	0.008046	0.003406
23	0.080085	0.002770	0.010957	0.004638
24	0.067288	0.002327	0.009206	0.003897
25	0.131517	0.004549	0.017994	0.007616
26	1.838276	0.063577	0.251510	0.106455
27	0.537486	0.018589	0.073538	0.031126
28	0.096034	0.003321	0.013139	0.005561
29	0.097008	0.003355	0.013273	0.005618
30	0.098355	0.003402	0.013457	0.005696
31	0.047440	0.001641	0.006491	0.002747
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999991	3.458510		

CARBON	BALANCE	7.421229 LB AT/MOLN2.	99.24 PERCENT
HYDROGEN	BALANCE	17.728071 LB AT/MOLN2.	94.83 PERCENT
OXYGEN	BALANCE	0.472595 LB AT/MOLN2.	88.89 PERCENT

PERCENT O2 REACT	95.0937	PERCENT C4 REACT	31.9453
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## VII - 6

RUN NO = 10 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.973531	0.034127	0.135397	0.053065
2	0.392798	0.013770	0.054630	0.021411
3	28.526563	1.000000	3.967416	1.554926
4	3.523195	0.123506	0.489999	0.192042
5	3.721398	0.130454	0.517564	0.202846
6	2.372449	0.083166	0.329955	0.129317
7	1.926073	0.067519	0.267874	0.104986
8	6.152494	0.215676	0.855676	0.335360
9	0.704589	0.024699	0.097993	0.038406
10	7.079269	0.248164	0.984570	0.385877
11	0.139092	0.004876	0.019345	0.007582
12	34.984476	1.226382	4.865569	1.906933
13	1.730651	0.060668	0.240695	0.094334
14	1.404868	0.049248	0.195386	0.076577
15	0.891466	0.031250	0.123983	0.048592
16	0.688484	0.024135	0.095753	0.037528
17	0.078623	0.002756	0.010935	0.004286
18	1.064200	0.037306	0.148007	0.058007
19	0.094658	0.003318	0.013165	0.005160
20	0.097083	0.003403	0.013502	0.005292
21	0.000000	0.000000	0.000000	0.000000
22	0.064909	0.002275	0.009027	0.003538
23	0.080110	0.002808	0.011142	0.004367
24	0.062522	0.002192	0.008695	0.003408
25	0.150099	0.005262	0.020875	0.008182
26	2.166763	0.075956	0.301349	0.118106
27	0.566504	0.019859	0.078788	0.030879
28	0.096817	0.003394	0.013465	0.005277
29	0.098094	0.003439	0.013643	0.005347
30	0.104043	0.003647	0.014470	0.005671
31	0.064187	0.002250	0.008927	0.003499
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.505504
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CARBON	BALANCE	7.420316 LB AT/MOLN2.	99.23 PERCENT
HYDROGEN	BALANCE	17.692138 LB AT/MOLN2.	94.64 PERCENT
OXYGEN	BALANCE	0.500982 LB AT/MOLN2.	94.23 PERCENT

PERCENT O2 REACT	94.8200	PERCENT C4 REACT	34.4005
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## VII - 7

RUN NO = 10 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.040903	0.036495	0.144975	0.057619
2	0.401969	0.014093	0.055985	0.022251
3	28.522192	1.000000	3.972517	1.578839
4	3.426980	0.120151	0.477303	0.189700
5	3.646785	0.127858	0.507917	0.201867
6	2.425811	0.085050	0.337862	0.134280
7	1.921380	0.067364	0.267606	0.106358
8	5.927909	0.207835	0.825628	0.328138
9	0.713686	0.025022	0.099401	0.039506
10	7.036168	0.246691	0.979984	0.389485
11	0.155755	0.005461	0.021693	0.008622
12	35.256945	1.236123	4.910520	1.951640
13	1.720829	0.060333	0.239674	0.095256
14	1.361742	0.047743	0.189661	0.075379
15	0.918975	0.032220	0.127993	0.050870
16	0.738271	0.025884	0.102825	0.040867
17	0.084303	0.002956	0.011742	0.004667
18	1.022632	0.035854	0.142430	0.056608
19	0.102970	0.003610	0.014341	0.005700
20	0.110648	0.003879	0.015411	0.006125
21	0.000000	0.000000	0.000000	0.000000
22	0.073508	0.002577	0.010238	0.004069
23	0.075873	0.002660	0.010567	0.004200
24	0.068374	0.002397	0.009523	0.003785
25	0.152895	0.005361	0.021295	0.008463
26	2.139743	0.075020	0.298019	0.118445
27	0.601537	0.021090	0.083781	0.033298
28	0.091405	0.003205	0.012731	0.005060
29	0.092260	0.003235	0.012850	0.005107
30	0.108934	0.003819	0.015172	0.006030
31	0.058629	0.002056	0.008166	0.003245
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999999	3.506042
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CARBON	BALANCE	7.440756 LB AT/MOLN2.	99.50 PERCENT
HYDROGEN	BALANCE	17.767363 LB AT/MOLN2.	95.04 PERCENT
OXYGEN	BALANCE	0.499746 LB AT/MOLN2.	94.00 PERCENT

PERCENT O2 REACT	94.6983	PERCENT C4 REACT	33.8795
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RUN NO = 11

REACTOR ENTRANCE CONDITIONS

AIR = 2.03 LB/HR BUTANE = 9.43 LB/HR

TEMPERATURE = 705.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 6.3519 NITROGEN = 23.8951 BUTANE = 69.7530 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.9191 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2109 LB/CU FT

GAS VELOCITY = 7.09 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.38 SEC

REYNOLDS NUMBER = 6000







RUN NO = 11 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.273427	0.011661	0.068819	0.056885
2	2.259730	0.096375	0.568755	0.470126
3	23.447387	1.000000	5.901506	4.878119
4	0.848583	0.036191	0.213581	0.176544
5	0.193042	0.008233	0.048587	0.040161
6	0.290045	0.012370	0.073002	0.060342
7	1.101425	0.046974	0.277219	0.229146
8	2.051273	0.087484	0.516288	0.426758
9	0.067390	0.002874	0.016962	0.014020
10	0.717621	0.030606	0.180619	0.149298
11	0.202277	0.008627	0.050911	0.042083
12	63.639437	2.714138	16.017500	13.239888
13	1.128508	0.048129	0.284036	0.234781
14	0.868631	0.037046	0.218627	0.180715
15	0.439023	0.018724	0.110498	0.091337
16	0.321499	0.013712	0.080919	0.066886
17	0.000000	0.000000	0.000000	0.000000
18	0.804229	0.034299	0.202418	0.167316
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.907689	0.038712	0.228457	0.188840
27	0.259959	0.011087	0.065430	0.054083
28	0.088767	0.003786	0.022342	0.018467
29	0.090061	0.003841	0.022667	0.018737
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	4.264867		

CARBON	BALANCE	11.790731 LB AT/MOLN2.	100.98 PERCENT
HYDROGEN	BALANCE	29.030535 LB AT/MOLN2.	99.45 PERCENT
OXYGEN	BALANCE	0.447049 LB AT/MOLN2.	84.09 PERCENT

PERCENT O2 REACT	63.7448	PERCENT C4 REACT	7.0225
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## VII - 10

RUN NO = 11 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.713924	0.031454	0.125612	0.064501
2	0.349859	0.015414	0.061556	0.031609
3	22.697209	1.000000	3.993473	2.050616
4	1.833533	0.080782	0.322602	0.165653
5	1.658758	0.073082	0.291851	0.149863
6	1.330614	0.058625	0.234116	0.120216
7	1.048640	0.046201	0.184504	0.094741
8	4.011525	0.176741	0.705810	0.362428
9	0.277879	0.012243	0.048892	0.025105
10	3.419169	0.150643	0.601588	0.308910
11	0.159068	0.007008	0.027987	0.014371
12	55.187729	2.431476	9.710036	4.986024
13	1.242254	0.054732	0.218569	0.112233
14	1.052349	0.046365	0.185156	0.095076
15	0.605679	0.026685	0.106567	0.054721
16	0.344660	0.015185	0.060641	0.031139
17	0.021282	0.000938	0.003744	0.001923
18	1.106360	0.048744	0.194659	0.099956
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.034222	0.001508	0.006021	0.003092
23	0.108480	0.004779	0.019087	0.009801
24	0.090035	0.003967	0.015841	0.008134
25	0.170072	0.007493	0.029923	0.015365
26	1.775068	0.078206	0.312315	0.160371
27	0.475638	0.020956	0.083686	0.042972
28	0.124268	0.005475	0.021864	0.011227
29	0.109766	0.004836	0.019313	0.009917
30	0.051967	0.002290	0.009143	0.004695
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999998	4.405828		

CARBON	BALANCE	11.609811 LB AT/MOLN2.	99.43 PERCENT
HYDROGEN	BALANCE	28.416213 LB AT/MOLN2.	97.34 PERCENT
OXYGEN	BALANCE	0.422630 LB AT/MOLN2.	79.49 PERCENT

PERCENT O2 REACT	94.2013	PERCENT C4 REACT	16.7056
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## VII - 11

RUN NO = 11 SAMPLE NO = 3

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.781695	0.034875	0.138513	0.064043
2	0.314750	0.014042	0.055773	0.025787
3	22.414251	1.000000	3.971716	1.836368
4	1.986232	0.088615	0.351952	0.162729
5	1.937953	0.086461	0.343398	0.158774
6	1.589601	0.070919	0.281671	0.130234
7	0.880675	0.039291	0.156052	0.072152
8	4.515036	0.201436	0.800046	0.369911
9	0.305056	0.013610	0.054055	0.024993
10	3.772422	0.168305	0.668458	0.309069
11	0.153060	0.006829	0.027122	0.012540
12	53.224471	2.374582	9.431163	4.360607
13	1.376716	0.061421	0.243949	0.112792
14	1.124944	0.050189	0.199336	0.092165
15	0.699313	0.031199	0.123916	0.057294
16	0.426154	0.019013	0.075513	0.034914
17	0.028614	0.001277	0.005070	0.002344
18	1.169337	0.052169	0.207202	0.095802
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.029154	0.001301	0.005166	0.002389
23	0.151434	0.006756	0.026834	0.012407
24	0.103116	0.004600	0.018272	0.008448
25	0.214101	0.009552	0.037938	0.017541
26	1.999571	0.089210	0.354316	0.163822
27	0.513531	0.022911	0.090996	0.042073
28	0.111140	0.004958	0.019694	0.009106
29	0.108785	0.004853	0.019276	0.008913
30	0.068894	0.003074	0.012208	0.005644
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999998	4.461447
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CARBON	BALANCE	11.602565 LB AT/MOLN2.	99.37 PERCENT
HYDROGEN	BALANCE	28.378516 LB AT/MOLN2.	97.22 PERCENT
OXYGEN	BALANCE	0.443578 LB AT/MOLN2.	83.43 PERCENT

PERCENT O2 REACT	94.7174	PERCENT C4 REACT	18.6546
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## VII - 12

RUN NO = 11 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.793488	0.035377	0.140289	0.061371
2	0.306223	0.013653	0.054140	0.023684
3	22.429698	1.000000	3.965575	1.734798
4	2.060998	0.091887	0.364385	0.159405
5	1.940272	0.086505	0.343040	0.150068
6	1.509248	0.067288	0.266835	0.116731
7	0.854970	0.038118	0.151159	0.066127
8	4.407927	0.196522	0.779322	0.340926
9	0.389689	0.017374	0.068897	0.030140
10	4.264291	0.190118	0.753927	0.329816
11	0.127136	0.005668	0.022478	0.009833
12	52.546028	2.342699	9.290148	4.064109
13	1.429443	0.063730	0.252726	0.110559
14	1.213489	0.054102	0.214545	0.093856
15	0.760256	0.033895	0.134413	0.058801
16	0.445995	0.019884	0.078852	0.034495
17	0.029929	0.001334	0.005291	0.002315
18	1.179072	0.052567	0.208460	0.091194
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.026360	0.001175	0.004660	0.002039
23	0.106621	0.004754	0.018851	0.008246
24	0.073662	0.003284	0.013023	0.005697
25	0.176851	0.007885	0.031267	0.013678
26	2.134383	0.095159	0.377359	0.165081
27	0.519594	0.023165	0.091864	0.040187
28	0.103015	0.004593	0.018213	0.007968
29	0.099253	0.004425	0.017548	0.007677
30	0.072117	0.003215	0.012750	0.005578
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	4.458374
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CARBON	BALANCE	11.547966 LB AT/MOLN2.	98.90 PERCENT
HYDROGEN	BALANCE	28.209609 LB AT/MOLN2.	96.64 PERCENT
OXYGEN	BALANCE	0.448254 LB AT/MOLN2.	84.31 PERCENT

PERCENT O2 REACT	94.8640	PERCENT C4 REACT	19.7468
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## VII - 13

RUN NO = 11 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.866484	0.039102	0.155447	0.070863
2	0.316307	0.014274	0.056745	0.025868
3	22.159377	1.000000	3.975375	1.812245
4	2.127681	0.096017	0.381704	0.174007
5	2.092041	0.094409	0.375310	0.171092
6	1.762700	0.079546	0.316227	0.144158
7	0.809973	0.036552	0.145309	0.066241
8	4.365414	0.197001	0.783152	0.357014
9	0.340639	0.015372	0.061110	0.027858
10	4.158683	0.187671	0.746065	0.340107
11	0.167771	0.007571	0.030098	0.013721
12	52.458625	2.367333	9.411037	4.290188
13	1.487994	0.067150	0.266945	0.121692
14	1.190967	0.053746	0.213659	0.097400
15	0.730020	0.032944	0.130965	0.059703
16	0.503278	0.022712	0.090288	0.041159
17	0.034260	0.001546	0.006146	0.002802
18	1.222348	0.055162	0.219288	0.099966
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.036756	0.001659	0.006594	0.003006
23	0.105731	0.004771	0.018968	0.008647
24	0.074614	0.003367	0.013386	0.006102
25	0.156443	0.007060	0.028066	0.012794
26	1.998214	0.090175	0.358478	0.163419
27	0.529332	0.023887	0.094962	0.043290
28	0.114661	0.005174	0.020570	0.009377
29	0.117066	0.005283	0.021002	0.009574
30	0.072625	0.003277	0.013029	0.005939
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	4.512762		

CARBON	BALANCE	11.709685 LB AT/MOLN2.	100.28 PERCENT
HYDROGEN	BALANCE	28.616109 LB AT/MOLN2.	98.03 PERCENT
OXYGEN	BALANCE	0.451483 LB AT/MOLN2.	84.92 PERCENT

PERCENT O2 REACT	94.6302	PERCENT C4 REACT	18.9029
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RUN NO = 12

REACTOR ENTRANCE CONDITIONS

AIR = 2.38 LB/HR BUTANE = 11.20 LB/HR

TEMPERATURE = 704.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 6.2946 NITROGEN = 23.6798 BUTANE = 70.0256 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.9572 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2114 LB/CU FT

GAS VELOCITY = 8.38 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.16 SEC

REYNOLDS NUMBER = 7129



## VII - 15

RUN NO = 12 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	4.742658	0.199591	3.013522	3.942011
3	23.761883	1.000000	15.098487	19.750448
4	0.204320	0.008599	0.129827	0.169827
5	0.047675	0.002006	0.030293	0.039626
6	0.060153	0.002531	0.038222	0.049998
7	0.276102	0.011620	0.175437	0.229491
8	0.255650	0.010759	0.162442	0.212492
9	0.000000	0.000000	0.000000	0.000000
10	0.093456	0.003933	0.059383	0.077679
11	0.222585	0.009367	0.141432	0.185009
12	69.065351	2.906561	43.884665	57.405873
13	0.273421	0.011507	0.173734	0.227263
14	0.139039	0.005851	0.088347	0.115567
15	0.071059	0.002990	0.045151	0.059063
16	0.060609	0.002551	0.038511	0.050377
17	0.000000	0.000000	0.000000	0.000000
18	0.211190	0.008888	0.134192	0.175538
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.336995	0.014182	0.214129	0.280104
27	0.177859	0.007485	0.113013	0.147833
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	100.000001	4.208421
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CARBON	BALANCE	11.834585 LB AT/MOLN2.	100.05 PERCENT
HYDROGEN	BALANCE	29.512999 LB AT/MOLN2.	99.80 PERCENT
OXYGEN	BALANCE	0.467116 LB AT/MOLN2.	87.86 PERCENT

PERCENT O2 REACT	24.9158	PERCENT C4 REACT	1.7122
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## VII - 16

RUN NO = 12 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.412019	0.018650	0.089830	0.053971
2	1.286009	0.058210	0.280379	0.168457
3	22.092500	1.000000	4.816664	2.893934
4	1.789935	0.081020	0.390246	0.234467
5	1.392288	0.063021	0.303550	0.182378
6	0.868227	0.039300	0.189293	0.113731
7	1.036373	0.046911	0.225953	0.135756
8	3.072429	0.139071	0.669859	0.402463
9	0.190062	0.008603	0.041438	0.024896
10	2.714280	0.122860	0.591774	0.355548
11	0.175372	0.007938	0.038235	0.022972
12	57.697700	2.611642	12.579402	7.557919
13	1.296767	0.058697	0.282725	0.169866
14	1.083263	0.049033	0.236176	0.141899
15	0.675311	0.030567	0.147233	0.088460
16	0.400001	0.018106	0.087209	0.052397
17	0.025229	0.001142	0.005500	0.003305
18	1.045496	0.047324	0.227942	0.136951
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.071553	0.003239	0.015600	0.009373
22	0.000000	0.000000	0.000000	0.000000
23	0.068000	0.003078	0.014826	0.008907
24	0.117711	0.005328	0.025664	0.015419
25	0.125572	0.005684	0.027377	0.016449
26	1.683042	0.076182	0.366941	0.220464
27	0.448735	0.020312	0.097834	0.058781
28	0.087925	0.003980	0.019170	0.011517
29	0.107159	0.004850	0.023363	0.014037
30	0.037046	0.001677	0.008077	0.004853
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	4.526423		

CARBON	BALANCE	12.149767 LB AT/MOLN2.	102.71 PERCENT
HYDROGEN	BALANCE	29.758449 LB AT/MOLN2.	100.63 PERCENT
OXYGEN	BALANCE	0.508349 LB AT/MOLN2.	95.62 PERCENT

PERCENT O2 REACT	78.1019	PERCENT C4 REACT	11.6851
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## VII - 17

RUN NO = 12 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.652150	0.029313	0.116252	0.054968
2	0.304163	0.013672	0.054220	0.025637
3	22.247750	1.000000	3.965875	1.875197
4	2.156781	0.096944	0.384467	0.181789
5	1.889175	0.084915	0.336764	0.159233
6	1.496476	0.067264	0.266761	0.126134
7	1.021577	0.045918	0.182106	0.086106
8	3.507366	0.157650	0.625222	0.295626
9	0.302840	0.013612	0.053984	0.025525
10	3.741446	0.168172	0.666949	0.315355
11	0.172045	0.007733	0.030669	0.014501
12	53.926657	2.423915	9.612945	4.545319
13	1.419690	0.063813	0.253073	0.119661
14	1.229653	0.055271	0.219197	0.103644
15	0.749296	0.033680	0.133569	0.063156
16	0.504740	0.022687	0.089975	0.042543
17	0.041931	0.001885	0.007475	0.003534
18	1.158143	0.052057	0.206450	0.097616
19	0.033364	0.001500	0.005947	0.002812
20	0.000000	0.000000	0.000000	0.000000
21	0.073995	0.003326	0.013190	0.006237
22	0.022708	0.001021	0.004048	0.001914
23	0.095274	0.004282	0.016984	0.008030
24	0.105692	0.004751	0.018841	0.008908
25	0.189365	0.008512	0.033756	0.015961
26	2.150284	0.096652	0.383309	0.181241
27	0.547711	0.024619	0.097635	0.046165
28	0.097255	0.004371	0.017337	0.008197
29	0.107725	0.004842	0.019203	0.009080
30	0.054756	0.002461	0.009761	0.004615
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999998	4.494836		

CARBON	BALANCE	11.781140 LB AT/MOLN2.	99.60 PERCENT
HYDROGEN	BALANCE	28.810010 LB AT/MOLN2.	97.42 PERCENT
OXYGEN	BALANCE	0.475037 LB AT/MOLN2.	89.35 PERCENT

PERCENT O2 REACT	94.8569	PERCENT C4 REACT	18.0332
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## VII - 18

RUN NO = 12 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.671201	0.030165	0.119681	0.052578
2	0.306655	0.013781	0.054679	0.024021
3	22.251236	1.000000	3.967604	1.743020
4	2.181140	0.098023	0.388918	0.170857
5	1.971684	0.088610	0.351570	0.154449
6	1.617711	0.072702	0.288453	0.126721
7	1.071498	0.048155	0.191058	0.083934
8	3.758717	0.168922	0.670214	0.294434
9	0.301934	0.013569	0.053838	0.023652
10	3.916935	0.176032	0.698426	0.306828
11	0.172975	0.007774	0.030843	0.013550
12	53.035272	2.383475	9.456685	4.154444
13	1.446256	0.064997	0.257881	0.113290
14	1.246143	0.056003	0.222199	0.097615
15	0.697013	0.031325	0.124284	0.054600
16	0.495668	0.022276	0.088382	0.038827
17	0.039537	0.001777	0.007050	0.003097
18	1.221928	0.054915	0.217881	0.095718
19	0.029182	0.001311	0.005203	0.002286
20	0.000000	0.000000	0.000000	0.000000
21	0.087630	0.003938	0.015625	0.006864
22	0.024912	0.001120	0.004442	0.001951
23	0.082163	0.003693	0.014650	0.006436
24	0.103440	0.004649	0.018444	0.008103
25	0.194990	0.008763	0.034769	0.015274
26	2.156338	0.096909	0.384495	0.168914
27	0.595803	0.026776	0.106237	0.046671
28	0.114959	0.005166	0.020498	0.009005
29	0.109433	0.004918	0.019513	0.008572
30	0.097652	0.004389	0.017412	0.007649
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.494132
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CARBON	BALANCE	11.708173 LB AT/MOLN2.	98.98 PERCENT
HYDROGEN	BALANCE	28.606546 LB AT/MOLN2.	96.74 PERCENT
OXYGEN	BALANCE	0.485673 LB AT/MOLN2.	91.35 PERCENT

PERCENT O2 REACT	94.8155	PERCENT C4 REACT	19.4007
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## VII - 19

RUN NO = 12 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.670121	0.030226	0.119937	0.052753
2	0.306161	0.013809	0.054796	0.024102
3	22.170543	1.000000	3.968043	1.745310
4	2.166407	0.097716	0.387740	0.170544
5	1.958964	0.088359	0.350612	0.154214
6	1.603628	0.072331	0.287014	0.126241
7	1.159686	0.052308	0.207559	0.091293
8	3.626034	0.163552	0.648981	0.285449
9	0.334742	0.015098	0.059911	0.026352
10	3.998582	0.180356	0.715659	0.314776
11	0.175711	0.007925	0.031448	0.013832
12	52.859632	2.384228	9.460719	4.161216
13	1.450215	0.065412	0.259557	0.114164
14	1.274749	0.057497	0.228152	0.100351
15	0.790201	0.035642	0.141429	0.062206
16	0.520656	0.023484	0.093186	0.040987
17	0.049201	0.002219	0.008806	0.003873
18	1.206187	0.054405	0.215881	0.094953
19	0.030694	0.001384	0.005494	0.002416
20	0.000000	0.000000	0.000000	0.000000
21	0.111121	0.005012	0.019888	0.008748
22	0.028515	0.001286	0.005103	0.002245
23	0.095384	0.004302	0.017072	0.007509
24	0.092036	0.004151	0.016472	0.007245
25	0.181827	0.008201	0.032543	0.014314
26	2.127819	0.095975	0.380833	0.167506
27	0.603637	0.027227	0.108038	0.047520
28	0.146824	0.006622	0.026278	0.011558
29	0.127678	0.005759	0.022852	0.010051
30	0.133051	0.006001	0.023813	0.010474
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	4.510489		

CARBON	BALANCE	11.759534 LB AT/MOLN2.	99.41 PERCENT
HYDROGEN	BALANCE	28.709971 LB AT/MOLN2.	97.09 PERCENT
OXYGEN	BALANCE	0.501720 LB AT/MOLN2.	94.37 PERCENT

PERCENT O2 REACT	94.8050	PERCENT C4 REACT	19.3753
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RUN NO = 13

REACTOR ENTRANCE CONDITIONS

AIR = 2.21 LB/HR BUTANE = 10.00 LB/HR

TEMPERATURE = 705.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 6.4688 NITROGEN = 24.3352 BUTANE = 69.1960 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.8435 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2102 LB/CU FT

GAS VELOCITY = 7.57 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.29 SEC

REYNOLDS NUMBER = 6369





## VII - 21

RUN NO = 13 SAMPLE NO = 1

PRGD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.076906	0.003144	0.012515	0.014928
2	0.357130	0.014600	0.058116	0.069321
3	24.461017	1.000000	3.980530	4.748009
4	0.648204	0.026499	0.105482	0.125820
5	0.152209	0.006223	0.024769	0.029545
6	0.156189	0.006385	0.025417	0.030317
7	4.054659	0.165760	0.659813	0.787030
8	1.092721	0.044672	0.177818	0.212103
9	0.000000	0.000000	0.000000	0.000000
10	0.548735	0.022433	0.089295	0.106512
11	0.166149	0.006792	0.027037	0.032250
12	64.401932	2.632840	10.480098	12.500746
13	0.792782	0.032410	0.129009	0.153883
14	0.684604	0.027988	0.111405	0.132885
15	0.155801	0.006369	0.025353	0.030242
16	0.130845	0.005349	0.021292	0.025398
17	0.000000	0.000000	0.000000	0.000000
18	0.518481	0.021196	0.084372	0.100640
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.046920	0.001918	0.007635	0.009107
24	0.058734	0.002401	0.009558	0.011401
25	0.083414	0.003410	0.013574	0.016191
26	1.134133	0.046365	0.184557	0.220141
27	0.149964	0.006131	0.024404	0.029109
28	0.059437	0.002430	0.009672	0.011537
29	0.069038	0.002822	0.011235	0.013401
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	4.088137		

CARBON	BALANCE	11.277111 LB AT/MOLN2.	99.15 PERCENT
HYDROGEN	BALANCE	27.592282 LB AT/MOLN2.	97.04 PERCENT
OXYGEN	BALANCE	0.485611 LB AT/MOLN2.	91.34 PERCENT

PERCENT O2 REACT	94.5076	PERCENT C4 REACT	7.4070
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## VII - 22

RUN NO = 13 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.390859	0.017115	0.067414	0.041914
2	0.272936	0.011951	0.047075	0.029268
3	22.837739	1.000000	3.938998	2.449004
4	1.683782	0.073728	0.290415	0.180560
5	1.330202	0.058246	0.229430	0.142644
6	1.150500	0.050377	0.198435	0.123374
7	2.226270	0.097482	0.383982	0.238734
8	3.435767	0.150443	0.592593	0.368434
9	0.247696	0.010846	0.042722	0.026562
10	3.254292	0.142496	0.561292	0.348974
11	0.146104	0.006397	0.025200	0.015667
12	55.612743	2.435125	9.591951	5.963629
13	1.481450	0.064869	0.255517	0.158863
14	1.132418	0.049585	0.195317	0.121435
15	0.536392	0.023487	0.092516	0.057520
16	0.426963	0.018695	0.073641	0.045785
17	0.000000	0.000000	0.000000	0.000000
18	0.787640	0.034489	0.135850	0.084463
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.166665	0.007298	0.028746	0.017872
24	0.221321	0.009691	0.038173	0.023733
25	0.143169	0.006269	0.024693	0.015353
26	1.828098	0.080047	0.315306	0.196036
27	0.389152	0.017040	0.067120	0.041731
28	0.133374	0.005840	0.023004	0.014302
29	0.123729	0.005418	0.021340	0.013268
30	0.040742	0.001784	0.007027	0.004369
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999995	4.378717		

CARBON	BALANCE	11.586579 LB AT/MOLN2.	101.87 PERCENT
HYDROGEN	BALANCE	28.197229 LB AT/MOLN2.	99.17 PERCENT
OXYGEN	BALANCE	0.502652 LB AT/MOLN2.	94.55 PERCENT

PERCENT O2 REACT	95.5041	PERCENT C4 REACT	14.3603
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## VII - 23

RUN NO = 13 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.580780	0.025108	0.098572	0.046004
2	0.256995	0.011110	0.043618	0.020357
3	23.131645	1.000000	3.925992	1.832274
4	2.000465	0.086482	0.339527	0.158458
5	1.873016	0.080972	0.317896	0.148363
6	1.388140	0.060010	0.235600	0.109956
7	1.491144	0.064463	0.253083	0.118115
8	3.731963	0.161336	0.633403	0.295612
9	0.298879	0.012921	0.050727	0.023674
10	3.916528	0.169315	0.664728	0.310231
11	0.143915	0.006222	0.024426	0.011400
12	53.149219	2.297684	9.020691	4.209988
13	1.523921	0.065880	0.258646	0.120711
14	1.316236	0.056902	0.223397	0.104260
15	0.501281	0.021671	0.085079	0.039707
16	0.401672	0.017365	0.068173	0.031817
17	0.029457	0.001273	0.005000	0.002333
18	0.983419	0.042514	0.166910	0.077897
19	0.018128	0.000784	0.003077	0.001436
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.016635	0.000719	0.002823	0.001318
23	0.127289	0.005503	0.021604	0.010083
24	0.157694	0.006817	0.026764	0.012491
25	0.156597	0.006770	0.026578	0.012404
26	1.830762	0.079145	0.310724	0.145016
27	0.606706	0.026228	0.102972	0.048058
28	0.141203	0.006104	0.023965	0.011185
29	0.134014	0.005794	0.022745	0.010615
30	0.092303	0.003990	0.015666	0.007311
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999999	4.323082		

CARBON	BALANCE	11.239846 LB AT/MOLN2.	98.82 PERCENT
HYDROGEN	BALANCE	27.381456 LB AT/MOLN2.	96.30 PERCENT
OXYGEN	BALANCE	0.459530 LB AT/MOLN2.	86.44 PERCENT

PERCENT O2 REACT	95.8205	PERCENT C4 REACT	19.1939
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## VII - 24

RUN NO = 13 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.563696	0.024318	0.095515	0.040027
2	0.260240	0.011227	0.044096	0.018479
3	23.180435	1.000000	3.927790	1.646016
4	2.098202	0.090516	0.355528	0.148991
5	1.981287	0.085472	0.335718	0.140689
6	1.734403	0.074822	0.293884	0.123158
7	1.282885	0.055343	0.217377	0.091096
8	3.969867	0.171259	0.672671	0.281896
9	0.293051	0.012642	0.049656	0.020809
10	4.338288	0.187153	0.735098	0.308057
11	0.155581	0.006712	0.026362	0.011048
12	51.829753	2.235927	8.782251	3.680371
13	1.524149	0.065752	0.258258	0.108228
14	1.353504	0.058390	0.229343	0.096111
15	0.516688	0.022290	0.087550	0.036689
16	0.432612	0.018663	0.073304	0.030719
17	0.041453	0.001788	0.007024	0.002944
18	1.060779	0.045762	0.179743	0.075325
19	0.020488	0.000884	0.003472	0.001455
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.012609	0.000544	0.002137	0.000895
23	0.095057	0.004101	0.016107	0.006750
24	0.131474	0.005672	0.022277	0.009336
25	0.141903	0.006122	0.024045	0.010076
26	1.964332	0.084741	0.332845	0.139485
27	0.652473	0.028148	0.110558	0.046331
28	0.129969	0.005607	0.022022	0.009229
29	0.128138	0.005528	0.021712	0.009099
30	0.106690	0.004603	0.018078	0.007576
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999998	4.313983
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CARBON	BALANCE	11.107843 LB AT/MOLN2.	97.66 PERCENT
HYDROGEN	BALANCE	27.057410 LB AT/MOLN2.	95.16 PERCENT
OXYGEN	BALANCE	0.454891 LB AT/MOLN2.	85.56 PERCENT

PERCENT O2 REACT	95.7766	PERCENT C4 REACT	21.3658
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## VII - 25

RUN NO = 13 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.572717	0.025036	0.098447	0.045240
2	0.263450	0.011516	0.045286	0.020811
3	22.875957	1.000000	3.932265	1.807024
4	2.026782	0.088599	0.348394	0.160100
5	1.935572	0.084612	0.332715	0.152895
6	1.564093	0.068373	0.268860	0.123551
7	1.254136	0.054823	0.215580	0.099067
8	3.890360	0.170063	0.668734	0.307308
9	0.318443	0.013920	0.054739	0.025155
10	4.362285	0.190693	0.749856	0.344587
11	0.139987	0.006119	0.024063	0.011058
12	52.387273	2.290058	9.005117	4.138191
13	1.572169	0.068726	0.270248	0.124189
14	1.407117	0.061511	0.241877	0.111151
15	0.570156	0.024924	0.098007	0.045038
16	0.461886	0.020191	0.079396	0.036485
17	0.040473	0.001769	0.006957	0.003197
18	1.090903	0.047688	0.187521	0.086173
19	0.034425	0.001505	0.005918	0.002719
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.029387	0.001285	0.005052	0.002321
23	0.094640	0.004137	0.016268	0.007476
24	0.111892	0.004891	0.019234	0.008839
25	0.137658	0.006018	0.023663	0.010874
26	1.892156	0.082714	0.325252	0.149466
27	0.628898	0.027492	0.108104	0.049678
28	0.120523	0.005269	0.020717	0.009520
29	0.103674	0.004532	0.017821	0.008189
30	0.112994	0.004939	0.019423	0.008926
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	4.371401
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CARBON	BALANCE	11.351267 LB AT/MOLN2.	99.80 PERCENT
HYDROGEN	BALANCE	27.643369 LB AT/MOLN2.	97.22 PERCENT
OXYGEN	BALANCE	0.454072 LB AT/MOLN2.	85.41 PERCENT

PERCENT O2 REACT	95.6676	PERCENT C4 REACT	19.4621
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VII - 26

RUN NO = 14

REACTOR ENTRANCE CONDITIONS

AIR = 2.21 LB/HR BUTANE = 10.00 LB/HR

TEMPERATURE = 696.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 6.4688 NITROGEN = 24.3352 BUTANE = 69.1960 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.8435 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2118 LB/CU FT

GAS VELOCITY = 7.52 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.30 SEC

REYNOLDS NUMBER = 6413





## VII - 27

RUN NO = 14 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.731194	0.235131	7.661109	5.460367
3	24.374446	1.000000	32.582269	23.222635
4	0.176667	0.007248	0.236157	0.168318
5	0.000000	0.000000	0.000000	0.000000
6	0.021047	0.000863	0.028134	0.020052
7	0.168318	0.006906	0.224997	0.160364
8	0.089449	0.003670	0.119570	0.085222
9	0.000000	0.000000	0.000000	0.000000
10	0.078001	0.003200	0.104267	0.074315
11	0.214117	0.008784	0.286219	0.203999
12	68.258021	2.800393	91.243146	65.032497
13	0.192109	0.007882	0.256799	0.183031
14	0.183272	0.007519	0.244987	0.174612
15	0.000000	0.000000	0.000000	0.000000
16	0.000000	0.000000	0.000000	0.000000
17	0.000000	0.000000	0.000000	0.000000
18	0.181756	0.007457	0.242960	0.173167
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.199365	0.008179	0.266499	0.189944
27	0.132237	0.005425	0.176766	0.125988
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	4.102657
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CARBON	BALANCE	11.356895 LB AT/MOLN2.	99.85 PERCENT
HYDROGEN	BALANCE	28.332774 LB AT/MOLN2.	99.64 PERCENT
OXYGEN	BALANCE	0.512383 LB AT/MOLN2.	96.38 PERCENT

PERCENT O2 REACT	11.5459	PERCENT C4 REACT	1.5144
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RUN NO = 14 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.310393	0.013376	0.055399	0.031926
2	0.565659	0.024376	0.100959	0.058182
3	23.205304	1.000000	4.141704	2.386841
4	1.565162	0.067448	0.279352	0.160989
5	0.932799	0.040198	0.166487	0.095945
6	0.715716	0.030843	0.127742	0.073617
7	1.402343	0.060432	0.250291	0.144242
8	3.249674	0.140040	0.580005	0.334254
9	0.178018	0.007671	0.031773	0.018311
10	2.230361	0.096114	0.398077	0.229410
11	0.183288	0.007899	0.032713	0.018853
12	56.261038	2.424490	10.041523	5.786874
13	1.547085	0.066669	0.276125	0.159129
14	1.343390	0.057892	0.239770	0.138178
15	0.934285	0.040262	0.166752	0.096098
16	0.582632	0.025108	0.103989	0.059928
17	0.019475	0.000839	0.003476	0.002003
18	1.284700	0.055362	0.229294	0.132141
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.054558	0.002351	0.009738	0.005612
22	0.000000	0.000000	0.000000	0.000000
23	0.086906	0.003745	0.015511	0.008939
24	0.100459	0.004329	0.017930	0.010333
25	0.158011	0.006809	0.028202	0.016253
26	1.848437	0.079656	0.329911	0.190126
27	0.744098	0.032066	0.132807	0.076536
28	0.199484	0.008596	0.035604	0.020518
29	0.179968	0.007755	0.032121	0.018511
30	0.083765	0.003610	0.014950	0.008616
31	0.032996	0.001422	0.005889	0.003394
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.309359
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CARBON	BALANCE	11.447015 LB AT/MOLN2.	100.64 PERCENT
HYDROGEN	BALANCE	27.937884 LB AT/MOLN2.	98.25 PERCENT
OXYGEN	BALANCE	0.505786 LB AT/MOLN2.	95.14 PERCENT

PERCENT O2 REACT	90.8299	PERCENT C4 REACT	14.7343
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## VII - 29

RUN NO = 14 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.493873	0.021541	0.085233	0.039375
2	0.300268	0.013096	0.051820	0.023940
3	22.927525	1.000000	3.956848	1.827950
4	2.045653	0.089223	0.353040	0.163094
5	1.627989	0.071006	0.280960	0.129795
6	1.381884	0.060272	0.238487	0.110174
7	1.483009	0.064682	0.255939	0.118236
8	3.823028	0.166744	0.659781	0.304800
9	0.270943	0.011817	0.046760	0.021602
10	3.559111	0.155233	0.614234	0.283758
11	0.170500	0.007436	0.029425	0.013594
12	52.650613	2.296393	9.086480	4.197692
13	1.647656	0.071864	0.284354	0.131363
14	1.523220	0.066436	0.262878	0.121442
15	0.894387	0.039009	0.154354	0.071307
16	0.567182	0.024738	0.097885	0.045220
17	0.041323	0.001802	0.007132	0.003295
18	1.114431	0.048607	0.192329	0.088851
19	0.021580	0.000941	0.003724	0.001721
20	0.000000	0.000000	0.000000	0.000000
21	0.091559	0.003993	0.015801	0.007300
22	0.000000	0.000000	0.000000	0.000000
23	0.080150	0.003496	0.013832	0.006390
24	0.091936	0.004010	0.015866	0.007330
25	0.163039	0.007111	0.028137	0.012999
26	1.758414	0.076694	0.303468	0.140194
27	0.768689	0.033527	0.132661	0.061286
28	0.179217	0.007817	0.030929	0.014289
29	0.172672	0.007531	0.029800	0.013767
30	0.101068	0.004408	0.017442	0.008058
31	0.049087	0.002141	0.008471	0.003914
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999999	4.361570
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CARBON	BALANCE	11.353991 LB AT/MOLN2.	99.83 PERCENT
HYDROGEN	BALANCE	27.594059 LB AT/MOLN2.	97.04 PERCENT
OXYGEN	BALANCE	0.503869 LB AT/MOLN2.	94.78 PERCENT

PERCENT O2 REACT	95.0733	PERCENT C4 REACT	19.2393
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## VII - 30

RUN NO = 14 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.586759	0.025637	0.101549	0.041507
2	0.305778	0.013360	0.052920	0.021631
3	22.886861	1.000000	3.960987	1.619018
4	2.113164	0.092331	0.365721	0.149485
5	1.837309	0.080278	0.317980	0.129971
6	1.571595	0.068668	0.271993	0.111175
7	1.515157	0.066202	0.262225	0.107182
8	4.340865	0.189666	0.751265	0.307073
9	0.294463	0.012866	0.050962	0.020830
10	3.911202	0.170893	0.676905	0.276679
11	0.166476	0.007274	0.028812	0.011777
12	50.941475	2.225796	8.816347	3.603602
13	1.607941	0.070256	0.278283	0.113746
14	1.622759	0.070904	0.280848	0.114794
15	0.896223	0.039159	0.155108	0.063399
16	0.606539	0.026502	0.104973	0.042907
17	0.041640	0.001819	0.007207	0.002946
18	1.030043	0.045006	0.178268	0.072865
19	0.036088	0.001577	0.006246	0.002553
20	0.000000	0.000000	0.000000	0.000000
21	0.130228	0.005690	0.022538	0.009212
22	0.000000	0.000000	0.000000	0.000000
23	0.085016	0.003715	0.014713	0.006014
24	0.087558	0.003826	0.015153	0.006194
25	0.161640	0.007063	0.027975	0.011434
26	1.858836	0.081218	0.321705	0.131494
27	0.796177	0.034788	0.137793	0.056322
28	0.199602	0.008721	0.034545	0.014120
29	0.173501	0.007581	0.030028	0.012273
30	0.136376	0.005959	0.023602	0.009647
31	0.058738	0.002566	0.010166	0.004155
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999998	4.369319
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CARBON	BALANCE	11.232142 LB AT/MOLN2.	98.75 PERCENT
HYDROGEN	BALANCE	27.264482 LB AT/MOLN2.	95.89 PERCENT
OXYGEN	BALANCE	0.517558 LB AT/MOLN2.	97.35 PERCENT

PERCENT O2 REACT	94.9739	PERCENT C4 REACT	21.7221
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## VII - 31

RUN NO = 14 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.554912	0.024674	0.097908	0.042628
2	0.310519	0.013807	0.054788	0.023854
3	22.489415	1.000000	3.968011	1.727643
4	2.119418	0.094241	0.373948	0.162814
5	1.851761	0.082339	0.326723	0.142253
6	1.677069	0.074571	0.295900	0.128833
7	1.513080	0.067280	0.266966	0.116235
8	4.315834	0.191905	0.761482	0.331544
9	0.362391	0.016114	0.063940	0.027839
10	4.116231	0.183030	0.726264	0.316210
11	0.164893	0.007332	0.029094	0.012667
12	50.930223	2.264631	8.986080	3.912473
13	1.631696	0.072554	0.287895	0.125347
14	1.542282	0.068578	0.272119	0.118479
15	0.890112	0.039579	0.157051	0.068379
16	0.588240	0.026156	0.103788	0.045189
17	0.038047	0.001692	0.006713	0.002923
18	0.999098	0.044425	0.176280	0.076751
19	0.043900	0.001952	0.007746	0.003372
20	0.000000	0.000000	0.000000	0.000000
21	0.128257	0.005703	0.022630	0.009853
22	0.038725	0.001722	0.006833	0.002975
23	0.073624	0.003274	0.012990	0.005656
24	0.070274	0.003125	0.012399	0.005398
25	0.222560	0.009896	0.039268	0.017097
26	1.943542	0.086420	0.342917	0.149303
27	0.849345	0.037766	0.149858	0.065247
28	0.180372	0.008020	0.031825	0.013856
29	0.171942	0.007645	0.030337	0.013209
30	0.122180	0.005433	0.021557	0.009386
31	0.060063	0.002671	0.010598	0.004614
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	4.446536
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CARBON	BALANCE	11.467072 LB AT/MOLN2.	100.82 PERCENT
HYDROGEN	BALANCE	27.851597 LB AT/MOLN2.	97.95 PERCENT
OXYGEN	BALANCE	0.530826 LB AT/MOLN2.	99.85 PERCENT

PERCENT O2 REACT	94.8058	PERCENT C4 REACT	20.3563
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VII - 32

RUN NO = 15

REACTOR ENTRANCE CONDITIONS

AIR = 2.21 LB/HR BUTANE = 10.05 LB/HR

TEMPERATURE = 727.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 6.4465 NITROGEN = 24.2513 BUTANE = 69.3022 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.8577 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2064 LB/CU FT

GAS VELOCITY = 7.74 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.26 SEC

REYNOLDS NUMBER = 6294



VII - 33

RUN NO = 15 SAMPLE NO = 1

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.388593	0.016143	0.065561	0.048531
2	0.471784	0.019599	0.079597	0.058921
3	24.072331	1.000000	4.061339	3.006387
4	1.614819	0.067082	0.272443	0.201674
5	0.764592	0.031762	0.128997	0.095490
6	0.516442	0.021454	0.087131	0.064498
7	1.716841	0.071320	0.289655	0.214416
8	1.361699	0.056567	0.229738	0.170062
9	0.066613	0.002767	0.011239	0.008319
10	1.352354	0.056179	0.228161	0.168895
11	0.198535	0.008247	0.033496	0.024795
12	60.783748	2.525046	10.255070	7.591265
13	1.013881	0.042118	0.171056	0.126623
14	0.862128	0.035814	0.145453	0.107671
15	0.625319	0.025977	0.105500	0.078096
16	0.386740	0.016066	0.065248	0.048300
17	0.024312	0.001010	0.004102	0.003036
18	1.538500	0.063912	0.259566	0.192143
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.088504	0.003677	0.014932	0.011053
24	0.059367	0.002466	0.010016	0.007414
25	0.060426	0.002510	0.010195	0.007547
26	1.275115	0.052970	0.215130	0.159249
27	0.474964	0.019731	0.080133	0.059318
28	0.113607	0.004719	0.019167	0.014188
29	0.109601	0.004553	0.018491	0.013688
30	0.059191	0.002459	0.009986	0.007392
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999998 4.154147

CARBON	BALANCE	11.243793 LB AT/MOLN2.	98.36 PERCENT
HYDROGEN	BALANCE	27.578981 LB AT/MOLN2.	96.51 PERCENT
OXYGEN	BALANCE	0.447958 LB AT/MOLN2.	84.26 PERCENT

PERCENT O2 REACT 92.6272 PERCENT C4 REACT 11.6397







RUN NO = 15 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.521812	0.022470	0.089043	0.062732
2	0.312753	0.013468	0.053369	0.037599
3	23.222243	1.000000	3.962672	2.791770
4	1.960460	0.084422	0.334535	0.235686
5	1.247853	0.053735	0.212935	0.150016
6	0.815759	0.035128	0.139202	0.098070
7	1.361016	0.058608	0.232245	0.163621
8	1.807704	0.077844	0.308469	0.217321
9	0.181137	0.007800	0.030909	0.021776
10	2.071102	0.089186	0.353415	0.248987
11	0.189007	0.008139	0.032252	0.022722
12	58.043432	2.499476	9.904603	6.977961
13	1.203777	0.051837	0.205414	0.144718
14	1.004416	0.043252	0.171395	0.120751
15	0.622518	0.026807	0.106227	0.074839
16	0.423009	0.018216	0.072183	0.050854
17	0.029030	0.001250	0.004954	0.003490
18	1.544939	0.066528	0.263630	0.185732
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.089621	0.003859	0.015293	0.010774
24	0.063400	0.002730	0.010819	0.007622
25	0.089767	0.003866	0.015318	0.010792
26	2.307044	0.099346	0.393677	0.277352
27	0.571237	0.024599	0.097477	0.068674
28	0.125997	0.005426	0.021500	0.015147
29	0.113902	0.004905	0.019436	0.013693
30	0.077071	0.003319	0.013152	0.009265
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.306216
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CARBON	BALANCE	11.451140 LB AT/MOLN2.	100.18 PERCENT
HYDROGEN	BALANCE	28.134477 LB AT/MOLN2.	98.45 PERCENT
OXYGEN	BALANCE	0.488174 LB AT/MOLN2.	91.82 PERCENT

PERCENT O2 REACT	94.9335	PERCENT C4 REACT	12.5345
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## VII - 35

RUN NO = 15 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.619201	0.026847	0.106596	0.071357
2	0.322058	0.013964	0.055443	0.037114
3	23.063818	1.000000	3.970475	2.657899
4	2.136312	0.092626	0.367770	0.246191
5	1.455040	0.063088	0.250488	0.167680
6	0.923828	0.040055	0.159039	0.106463
7	1.096356	0.047536	0.188740	0.126345
8	2.051282	0.088939	0.353132	0.236392
9	0.213425	0.009254	0.036741	0.024595
10	2.264173	0.098170	0.389781	0.260926
11	0.182477	0.007912	0.031414	0.021029
12	57.231352	2.481434	9.852474	6.595402
13	1.223687	0.053057	0.210660	0.141019
14	1.095728	0.047509	0.188631	0.126273
15	0.638820	0.027698	0.109974	0.073618
16	0.425030	0.018428	0.073170	0.048981
17	0.030113	0.001306	0.005184	0.003470
18	1.418607	0.061508	0.244216	0.163482
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.023202	0.001006	0.003994	0.002674
22	0.000000	0.000000	0.000000	0.000000
23	0.086283	0.003741	0.014854	0.009943
24	0.061104	0.002649	0.010519	0.007042
25	0.113357	0.004915	0.019515	0.013063
26	2.397758	0.103962	0.412778	0.276320
27	0.586972	0.025450	0.101048	0.067643
28	0.129243	0.005604	0.022249	0.014894
29	0.134054	0.005812	0.023078	0.015449
30	0.076726	0.003327	0.013208	0.008842
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	4.335795
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CARBON	BALANCE	11.473919 LB AT/MOLN2.	100.38 PERCENT
HYDROGEN	BALANCE	28.204623 LB AT/MOLN2.	98.70 PERCENT
OXYGEN	BALANCE	0.478719 LB AT/MOLN2.	90.04 PERCENT

PERCENT O2 REACT	94.7470	PERCENT C4 REACT	13.1659
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## VII - 36

RUN NO = 15 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.567668	0.024452	0.101903	0.057323
2	0.600634	0.025872	0.107821	0.060652
3	23.215891	1.000000	4.167516	2.344346
4	2.119631	0.091301	0.380498	0.214041
5	1.435266	0.061823	0.257647	0.144934
6	0.989031	0.042601	0.177542	0.099873
7	1.127105	0.048549	0.202328	0.113815
8	2.125173	0.091540	0.381493	0.214600
9	0.254004	0.010941	0.045597	0.025649
10	2.341065	0.100839	0.420248	0.236401
11	0.182876	0.007877	0.032828	0.018467
12	56.440460	2.431113	10.131702	5.699371
13	1.188500	0.051193	0.213349	0.120015
14	1.128141	0.048593	0.202514	0.113920
15	0.633743	0.027298	0.113764	0.063996
16	0.400498	0.017251	0.071894	0.040442
17	0.029138	0.001255	0.005231	0.002942
18	1.472607	0.063431	0.264350	0.148704
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.059387	0.002558	0.010661	0.005997
22	0.000000	0.000000	0.000000	0.000000
23	0.105036	0.004524	0.018855	0.010607
24	0.060629	0.002612	0.010884	0.006122
25	0.123790	0.005332	0.022222	0.012500
26	2.451682	0.105604	0.440105	0.247571
27	0.617646	0.026604	0.110874	0.062370
28	0.134895	0.005810	0.024215	0.013622
29	0.110367	0.004754	0.019812	0.011145
30	0.085145	0.003668	0.015284	0.008598
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.307394
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CARBON	BALANCE	11.303897 LB AT/MOLN2.	98.89 PERCENT
HYDROGEN	BALANCE	27.775749 LB AT/MOLN2.	97.20 PERCENT
OXYGEN	BALANCE	0.507030 LB AT/MOLN2.	95.37 PERCENT

PERCENT O2 REACT	90.2673	PERCENT C4 REACT	14.9268
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## VII - 37

RUN NO = 15 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.639078	0.027718	0.109850	0.070209
2	0.311218	0.013498	0.053495	0.034190
3	23.056520	1.000000	3.963147	2.532970
4	2.116281	0.091787	0.363764	0.232493
5	1.532826	0.066481	0.263475	0.168395
6	0.905387	0.039268	0.155625	0.099465
7	1.040884	0.045145	0.178916	0.114351
8	2.020269	0.087622	0.347261	0.221945
9	0.265283	0.011506	0.045599	0.029144
10	2.350865	0.101961	0.404086	0.258264
11	0.182361	0.007909	0.031346	0.020034
12	56.785392	2.462878	9.760746	6.238394
13	1.203388	0.052193	0.206848	0.132203
14	1.102486	0.047817	0.189504	0.121118
15	0.639297	0.027727	0.109888	0.070233
16	0.408100	0.017700	0.070148	0.044834
17	0.027679	0.001201	0.004758	0.003041
18	1.455885	0.063144	0.250250	0.159942
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.069330	0.003007	0.011917	0.007617
22	0.023629	0.001025	0.004062	0.002596
23	0.112503	0.004879	0.019338	0.012360
24	0.071405	0.003097	0.012274	0.007844
25	0.163641	0.007097	0.028128	0.017977
26	2.494317	0.108183	0.428744	0.274024
27	0.673848	0.029226	0.115827	0.074028
28	0.139101	0.006033	0.023910	0.015281
29	0.121496	0.005269	0.020884	0.013347
30	0.087540	0.003797	0.015047	0.009617
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.337168
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CARBON	BALANCE	11.446468 LB AT/MOLN2.	100.14 PERCENT
HYDROGEN	BALANCE	28.157663 LB AT/MOLN2.	98.53 PERCENT
OXYGEN	BALANCE	0.485226 LB AT/MOLN2.	91.27 PERCENT

PERCENT O2 REACT	94.9222	PERCENT C4 REACT	13.8152
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RUN NO = 16

REACTOR ENTRANCE CONDITIONS

AIR = 2.63 LB/HR BUTANE = 10.05 LB/HR

TEMPERATURE = 702.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 7.2488 NITROGEN = 27.2692 BUTANE = 65.4820 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.4013 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2060 LB/CU FT

GAS VELOCITY = 8.02 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.22 SEC

REYNOLDS NUMBER = 6467







RUN NO = 16 SAMPLE NO = 1

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.379019	0.014368	0.065797	0.039344
2	1.251567	0.047446	0.217269	0.129920
3	26.378575	1.000000	4.579248	2.738243
4	1.100386	0.041715	0.191024	0.114226
5	0.913347	0.034625	0.158554	0.094810
6	0.969532	0.036755	0.168308	0.100643
7	3.625423	0.137438	0.629363	0.376339
8	3.725852	0.141245	0.646798	0.386764
9	0.160807	0.006096	0.027916	0.016693
10	2.202110	0.083481	0.382280	0.228591
11	0.165091	0.006259	0.028659	0.017137
12	53.709826	2.036115	9.323879	5.575378
13	1.362603	0.051656	0.236544	0.141446
14	1.401233	0.053120	0.243250	0.145456
15	0.560005	0.021230	0.097215	0.058132
16	0.486244	0.018433	0.084411	0.050475
17	0.000000	0.000000	0.000000	0.000000
18	0.577295	0.021885	0.100217	0.059926
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.167039	0.006332	0.028997	0.017340
25	0.137234	0.005202	0.023823	0.014246
26	0.492086	0.018655	0.085425	0.051081
27	0.163673	0.006205	0.028413	0.016990
28	0.000000	0.000000	0.000000	0.000000
29	0.071056	0.002694	0.012335	0.007376
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999998	3.790955
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CARBON	BALANCE	9.576358 LB AT/MOLN2.	99.70 PERCENT
HYDROGEN	BALANCE	23.122969 LB AT/MOLN2.	96.29 PERCENT
OXYGEN	BALANCE	0.512120 LB AT/MOLN2.	96.33 PERCENT

PERCENT O2 REACT	82.1511	PERCENT C4 REACT	15.2083
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## VII - 40

RUN NO = 16 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.533148	0.020972	0.083103	0.035481
2	0.342242	0.013462	0.053346	0.022776
3	25.421887	1.000000	3.962589	1.691810
4	2.144941	0.084374	0.334339	0.142744
5	1.918653	0.075472	0.299066	0.127685
6	1.601077	0.062980	0.249565	0.106551
7	2.193674	0.086291	0.341935	0.145988
8	5.334994	0.209858	0.831582	0.355040
9	0.283512	0.011152	0.044192	0.018868
10	4.782126	0.188111	0.745405	0.318247
11	0.144820	0.005697	0.022574	0.009638
12	46.019466	1.810230	7.173197	3.062565
13	1.929307	0.075892	0.300727	0.128394
14	1.892007	0.074424	0.294913	0.125912
15	0.813339	0.031994	0.126778	0.054127
16	0.537658	0.021149	0.083806	0.035781
17	0.041410	0.001629	0.006455	0.002756
18	0.727041	0.028599	0.113326	0.048384
19	0.081038	0.003188	0.012632	0.005393
20	0.091168	0.003586	0.014211	0.006067
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.075973	0.002989	0.011842	0.005056
24	0.151675	0.005966	0.023642	0.010094
25	0.179361	0.007055	0.027958	0.011936
26	1.936554	0.076177	0.301857	0.128876
27	0.436360	0.017165	0.068017	0.029039
28	0.063015	0.002479	0.009822	0.004194
29	0.138827	0.005461	0.021639	0.009239
30	0.118854	0.004675	0.018526	0.007910
31	0.065879	0.002591	0.010269	0.004384
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.933618
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CARBON	BALANCE	9.547896 LB AT/MOLN2.	99.40 PERCENT
HYDROGEN	BALANCE	22.947248 LB AT/MOLN2.	95.56 PERCENT
OXYGEN	BALANCE	0.493767 LB AT/MOLN2.	92.88 PERCENT

PERCENT O2 REACT	94.9355	PERCENT C4 REACT	24.6150
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## VII - 41

RUN NO = 16 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.650639	0.026128	0.103593	0.041503
2	0.338739	0.013603	0.053933	0.021608
3	24.901860	1.000000	3.964795	1.588453
4	2.333754	0.093718	0.371573	0.148867
5	2.404713	0.096568	0.382871	0.153393
6	2.122934	0.085252	0.338007	0.135419
7	1.999519	0.080296	0.318357	0.127546
8	5.328977	0.213999	0.848463	0.339928
9	0.369719	0.014847	0.058865	0.023584
10	5.483425	0.220201	0.873054	0.349780
11	0.138691	0.005570	0.022082	0.008847
12	44.120361	1.771770	7.024704	2.814372
13	1.885998	0.075737	0.300283	0.120305
14	1.848847	0.074245	0.294368	0.117935
15	0.833736	0.033481	0.132745	0.053183
16	0.553917	0.022244	0.088193	0.035334
17	0.048090	0.001931	0.007657	0.003068
18	0.765431	0.030738	0.121870	0.048826
19	0.079284	0.003184	0.012623	0.005057
20	0.081315	0.003265	0.012947	0.005187
21	0.000000	0.000000	0.000000	0.000000
22	0.046970	0.001886	0.007478	0.002996
23	0.114864	0.004613	0.018288	0.007327
24	0.114785	0.004609	0.018276	0.007322
25	0.234898	0.009433	0.037400	0.014984
26	2.236230	0.089802	0.356045	0.142646
27	0.601489	0.024154	0.095767	0.038368
28	0.076642	0.003078	0.012203	0.004889
29	0.128117	0.005145	0.020398	0.008172
30	0.088241	0.003544	0.014049	0.005629
31	0.067823	0.002724	0.010798	0.004326
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	4.015764
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CARBON	BALANCE	9.612196 LB AT/MOLN2.	100.07 PERCENT
HYDROGEN	BALANCE	23.144500 LB AT/MOLN2.	96.38 PERCENT
OXYGEN	BALANCE	0.518345 LB AT/MOLN2.	97.50 PERCENT

PERCENT O2 REACT	94.8827	PERCENT C4 REACT	26.2166
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VII - 42

RUN NO = 16 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.739491	0.029628	0.117390	0.045577
2	0.335236	0.013431	0.053217	0.020662
3	24.959032	1.000000	3.962101	1.538295
4	2.399985	0.096157	0.380984	0.147918
5	2.431731	0.097429	0.386023	0.149874
6	2.167671	0.086849	0.344105	0.133600
7	1.947811	0.078040	0.309204	0.120049
8	5.428972	0.217515	0.861818	0.334603
9	0.383432	0.015362	0.060868	0.023632
10	5.566929	0.223043	0.883718	0.343105
11	0.137047	0.005491	0.021755	0.008447
12	43.709331	1.751243	6.938602	2.693929
13	1.801901	0.072194	0.286041	0.111056
14	1.876564	0.075186	0.297894	0.115658
15	0.800540	0.032074	0.127081	0.049340
16	0.559036	0.022398	0.088744	0.034455
17	0.046246	0.001853	0.007341	0.002850
18	0.816348	0.032708	0.129591	0.050314
19	0.076637	0.003071	0.012166	0.004723
20	0.080931	0.003243	0.012847	0.004988
21	0.000000	0.000000	0.000000	0.000000
22	0.050006	0.002004	0.007938	0.003082
23	0.105210	0.004215	0.016702	0.006484
24	0.096795	0.003878	0.015366	0.005966
25	0.224505	0.008995	0.035639	0.013837
26	2.202786	0.088256	0.349679	0.135764
27	0.684703	0.027433	0.108693	0.042200
28	0.076407	0.003061	0.012129	0.004709
29	0.125998	0.005048	0.020001	0.007766
30	0.093050	0.003728	0.014771	0.005735
31	0.075676	0.003032	0.012013	0.004664
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999999 4.006566

CARBON	BALANCE	9.547601 LB AT/MOLN2.	99.40 PERCENT
HYDROGEN	BALANCE	22.989490 LB AT/MOLN2.	95.74 PERCENT
OXYGEN	BALANCE	0.517170 LB AT/MOLN2.	97.28 PERCENT

PERCENT O2 REACT 94.9472 PERCENT C4 REACT 27.0714





## VII - 43

RUN NO = 16 SAMPLE NO = 5

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.774176	0.031280	0.123770	0.049406
2	0.324040	0.013093	0.051805	0.020679
3	24.749496	1.000000	3.956792	1.579438
4	2.356349	0.095208	0.376718	0.150375
5	2.409525	0.097357	0.385219	0.153769
6	2.128768	0.086013	0.340334	0.135851
7	1.896581	0.076631	0.303213	0.121034
8	5.394415	0.217961	0.862425	0.344255
9	0.417297	0.016861	0.066715	0.026631
10	5.637588	0.227786	0.901302	0.359774
11	0.135157	0.005461	0.021608	0.008625
12	43.761476	1.768176	6.996306	2.792724
13	1.809190	0.073100	0.289242	0.115457
14	1.834950	0.074141	0.293360	0.117101
15	0.849780	0.034335	0.135857	0.054230
16	0.560504	0.022647	0.089610	0.035770
17	0.053205	0.002150	0.008506	0.003395
18	0.809635	0.032713	0.129439	0.051668
19	0.082381	0.003329	0.013171	0.005257
20	0.064763	0.002617	0.010354	0.004133
21	0.000000	0.000000	0.000000	0.000000
22	0.049814	0.002013	0.007964	0.003179
23	0.099678	0.004027	0.015936	0.006361
24	0.073341	0.002963	0.011725	0.004680
25	0.238368	0.009631	0.038109	0.015212
26	2.285811	0.092358	0.365441	0.145874
27	0.789041	0.031881	0.126147	0.050354
28	0.101368	0.004096	0.016206	0.006469
29	0.148029	0.005981	0.023666	0.009447
30	0.097704	0.003948	0.015620	0.006235
31	0.067578	0.002730	0.010804	0.004313
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	4.040486
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CARBON	BALANCE	9.647138 LB AT/MOLN2.	100.44 PERCENT
HYDROGEN	BALANCE	23.251511 LB AT/MOLN2.	96.83 PERCENT
OXYGEN	BALANCE	0.524584 LB AT/MOLN2.	98.67 PERCENT

PERCENT O2 REACT	95.0746	PERCENT C4 REACT	26.3663
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RUN NO = 17

REACTOR ENTRANCE CONDITIONS

AIR = 2.65 LB/HR BUTANE = 10.15 LB/HR

TEMPERATURE = 681.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 7.2378 NITROGEN = 27.2277 BUTANE = 65.5345 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.4069 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2099 LB/CU FT

GAS VELOCITY = 7.95 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.23 SEC

REYNOLDS NUMBER = 6636



## VII - 45

RUN NO = 17 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.010957	0.257769	32.006684	11.466200
3	27.198584	1.000000	124.168004	44.482430
4	0.123592	0.004544	0.564226	0.202131
5	0.000000	0.000000	0.000000	0.000000
6	0.032635	0.001200	0.148988	0.053374
7	0.099932	0.003674	0.456214	0.163436
8	0.083914	0.003085	0.383085	0.137238
9	0.000000	0.000000	0.000000	0.000000
10	0.077684	0.002856	0.354647	0.127050
11	0.191094	0.007026	0.872392	0.312529
12	64.852919	2.384423	296.068992	106.064912
13	0.144221	0.005303	0.658405	0.235870
14	0.133448	0.004906	0.609220	0.218249
15	0.000000	0.000000	0.000000	0.000000
16	0.000000	0.000000	0.000000	0.000000
17	0.000000	0.000000	0.000000	0.000000
18	0.051019	0.001876	0.232915	0.083440
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	3.676662
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CARBON	BALANCE	9.635738 LB AT/MOLN2.	100.08 PERCENT
HYDROGEN	BALANCE	24.040337 LB AT/MOLN2.	99.88 PERCENT
OXYGEN	BALANCE	0.529307 LB AT/MOLN2.	99.56 PERCENT

PERCENT O2 REACT	3.0297	PERCENT C4 REACT	0.9340
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## VII - 46

RUN NO = 17 SAMPLE NO = 2

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.204431	0.190068	2.508978	3.047275
3	27.381980	1.000000	13.200442	16.032575
4	0.341577	0.012475	0.164669	0.199998
5	0.173946	0.006353	0.083857	0.101848
6	0.076186	0.002782	0.036728	0.044608
7	0.922173	0.033678	0.444566	0.539947
8	0.195977	0.007157	0.094478	0.114748
9	0.000000	0.000000	0.000000	0.000000
10	0.219977	0.008034	0.106048	0.128800
11	0.188200	0.006873	0.090729	0.110194
12	64.197884	2.344530	30.948838	37.588859
13	0.278036	0.010154	0.134037	0.162794
14	0.314560	0.011488	0.151645	0.184180
15	0.000000	0.000000	0.000000	0.000000
16	0.068791	0.002512	0.033163	0.040278
17	0.000000	0.000000	0.000000	0.000000
18	0.166001	0.006062	0.080027	0.097196
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.143298	0.005233	0.069082	0.083903
28	0.070329	0.002568	0.033904	0.041179
29	0.056655	0.002069	0.027312	0.033172
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.652037
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CARBON	BALANCE	9.634832 LB AT/MOLN2.	100.07 PERCENT
HYDROGEN	BALANCE	23.908902 LB AT/MOLN2.	99.33 PERCENT
OXYGEN	BALANCE	0.478412 LB AT/MOLN2.	89.99 PERCENT

PERCENT O2 REACT	28.4983	PERCENT C4 REACT	2.5914
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## VII - 47

RUN NO = 17 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.415077	0.016240	0.074890	0.041125
2	1.251679	0.048972	0.225834	0.124014
3	25.558973	1.000000	4.611470	2.532331
4	1.832543	0.071699	0.330636	0.181565
5	1.396986	0.054657	0.252051	0.138411
6	1.026967	0.040180	0.185290	0.101750
7	1.984735	0.077653	0.358095	0.196643
8	3.981584	0.155780	0.718376	0.394487
9	0.195790	0.007660	0.035325	0.019398
10	3.252247	0.127245	0.586786	0.322226
11	0.146306	0.005724	0.026397	0.014496
12	51.424918	2.012010	9.278326	5.095076
13	1.527827	0.059777	0.275658	0.151374
14	1.473062	0.057634	0.265777	0.145948
15	0.377190	0.014758	0.068054	0.037371
16	0.392421	0.015354	0.070803	0.038880
17	0.024784	0.000970	0.004472	0.002456
18	1.014458	0.039691	0.183033	0.100510
19	0.076872	0.003008	0.013870	0.007616
20	0.113024	0.004422	0.020392	0.011198
21	0.073759	0.002886	0.013308	0.007308
22	0.000000	0.000000	0.000000	0.000000
23	0.057890	0.002265	0.010445	0.005736
24	0.082572	0.003231	0.014898	0.008181
25	0.139538	0.005459	0.025176	0.013825
26	1.137493	0.044505	0.205232	0.112700
27	0.664666	0.026005	0.119922	0.065854
28	0.096843	0.003789	0.017473	0.009595
29	0.152124	0.005952	0.027447	0.015072
30	0.082368	0.003223	0.014861	0.008161
31	0.045310	0.001773	0.008175	0.004489
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.912520
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CARBON	BALANCE	9.847991 LB AT/MOLN2.	102.29 PERCENT
HYDROGEN	BALANCE	23.842333 LB AT/MOLN2.	99.06 PERCENT
OXYGEN	BALANCE	0.495375 LB AT/MOLN2.	93.18 PERCENT

PERCENT O2 REACT	81.5771	PERCENT C4 REACT	16.4067
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RUN NO = 17 SAMPLE NO = 4

PRGD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.656266	0.026077	0.103927	0.052387
2	0.375265	0.014911	0.059427	0.029956
3	25.166901	1.000000	3.985465	2.008975
4	2.101870	0.083517	0.332855	0.167784
5	2.056069	0.081697	0.325602	0.164128
6	1.473697	0.058557	0.233377	0.117639
7	2.538244	0.100856	0.401960	0.202618
8	4.192311	0.166580	0.663900	0.334656
9	0.252247	0.010023	0.039946	0.020136
10	4.567056	0.181471	0.723245	0.364570
11	0.140539	0.005584	0.022256	0.011219
12	48.047068	1.909137	7.608800	3.835410
13	1.479804	0.058800	0.234344	0.118127
14	1.452214	0.057703	0.229975	0.115925
15	0.559815	0.022244	0.088653	0.044688
16	0.431738	0.017155	0.068371	0.034464
17	0.042566	0.001691	0.006741	0.003398
18	0.926532	0.036815	0.146727	0.073961
19	0.091809	0.003648	0.014539	0.007329
20	0.134741	0.005354	0.021338	0.010756
21	0.078063	0.003102	0.012362	0.006231
22	0.030281	0.001203	0.004795	0.002417
23	0.101877	0.004048	0.016133	0.008132
24	0.112093	0.004454	0.017751	0.008948
25	0.269283	0.010700	0.042644	0.021496
26	1.485205	0.059014	0.235199	0.118558
27	0.789336	0.031364	0.125000	0.063010
28	0.136217	0.005413	0.021572	0.010874
29	0.178850	0.007107	0.028323	0.014277
30	0.077078	0.003063	0.012206	0.006153
31	0.054972	0.002184	0.008705	0.004388
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.973473
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CARBON	BALANCE	9.783617 LB AT/MOLN2.	101.62 PERCENT
HYDROGEN	BALANCE	23.608207 LB AT/MOLN2.	98.09 PERCENT
OXYGEN	BALANCE	0.523967 LB AT/MOLN2.	98.56 PERCENT

PERCENT O2 REACT	94.3906	PERCENT C4 REACT	20.6808
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RUN NO = 17 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.659703	0.026012	0.103136	0.046928
2	0.345275	0.013614	0.053979	0.024561
3	25.361722	1.000000	3.964969	1.804123
4	2.184642	0.086139	0.341540	0.155406
5	2.180686	0.085983	0.340921	0.155125
6	1.626626	0.064137	0.254301	0.115711
7	2.526262	0.099609	0.394948	0.179707
8	4.297137	0.169434	0.671801	0.305680
9	0.237400	0.009361	0.037114	0.016888
10	4.675116	0.184337	0.730892	0.332567
11	0.141501	0.005579	0.022122	0.010066
12	46.985567	1.852617	7.345571	3.342349
13	1.541015	0.060761	0.240917	0.109621
14	1.526709	0.060197	0.238681	0.108603
15	0.598637	0.023604	0.093589	0.042584
16	0.424312	0.016730	0.066336	0.030184
17	0.040337	0.001590	0.006306	0.002869
18	0.916889	0.036152	0.143344	0.065224
19	0.097900	0.003860	0.015305	0.006964
20	0.177575	0.007002	0.027762	0.012632
21	0.069328	0.002734	0.010839	0.004932
22	0.068150	0.002687	0.010654	0.004848
23	0.106435	0.004197	0.016640	0.007571
24	0.112347	0.004430	0.017564	0.007992
25	0.311233	0.012272	0.048657	0.022140
26	1.506982	0.059420	0.235597	0.107200
27	0.814959	0.032133	0.127408	0.057973
28	0.120845	0.004765	0.018893	0.008596
29	0.165218	0.006514	0.025830	0.011753
30	0.118534	0.004674	0.018531	0.008432
31	0.060963	0.002404	0.009531	0.004337
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.942950
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CARBON	BALANCE	9.620316 LB AT/MOLN2.	99.92 PERCENT
HYDROGEN	BALANCE	23.195254 LB AT/MOLN2.	96.37 PERCENT
OXYGEN	BALANCE	0.526882 LB AT/MOLN2.	99.10 PERCENT

PERCENT O2 REACT	94.8785	PERCENT C4 REACT	23.0290
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RUN NO = 18

REACTOR ENTRANCE CONDITIONS

AIR = 2.58 LB/HR BUTANE = 9.85 LB/HR

TEMPERATURE = 723.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 7.2531 NITROGEN = 27.2854 BUTANE = 65.4615 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.3991 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2024 LB/CU FT

GAS VELOCITY = 8.01 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.22 SEC

REYNOLDS NUMBER = 6240





VII - 51

RUN NO = 18 SAMPLE NO = 1

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.474655	0.018014	0.074978	0.051019
2	0.673436	0.025559	0.106378	0.072386
3	26.348589	1.000000	4.162087	2.832139
4	1.828362	0.069391	0.288813	0.196526
5	1.243991	0.047213	0.196504	0.133713
6	0.698282	0.026502	0.110302	0.075056
7	2.285662	0.086747	0.361049	0.245680
8	2.471368	0.093795	0.390383	0.265641
9	0.117483	0.004459	0.018558	0.012628
10	2.229633	0.084621	0.352198	0.239657
11	0.109984	0.004174	0.017373	0.011822
12	53.910448	2.046047	8.515825	5.794689
13	1.500328	0.056941	0.236995	0.161266
14	1.366160	0.051849	0.215802	0.146845
15	0.195857	0.007433	0.030938	0.021052
16	0.199788	0.007583	0.031559	0.021475
17	0.000000	0.000000	0.000000	0.000000
18	1.050096	0.039854	0.165876	0.112872
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.091146	0.003459	0.014398	0.009797
24	0.083002	0.003150	0.013111	0.008922
25	0.245616	0.009322	0.038798	0.026401
26	1.690627	0.064164	0.267056	0.181721
27	0.822983	0.031234	0.130000	0.088460
28	0.183544	0.006966	0.028993	0.019729
29	0.178964	0.006792	0.028270	0.019236
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999998 3.795270

CARBON	BALANCE	9.596188 LB AT/MOLN2.	100.00 PERCENT
HYDROGEN	BALANCE	23.382356 LB AT/MOLN2.	97.46 PERCENT
OXYGEN	BALANCE	0.473960 LB AT/MOLN2.	89.15 PERCENT

PERCENT O2 REACT 90.3851 PERCENT C4 REACT 14.7174





## VII - 52

RUN NO = 18 SAMPLE NO = 2

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.718356	0.028307	0.112115	0.053095
2	0.338639	0.013344	0.052852	0.025030
3	25.377619	1.000000	3.960729	1.875721
4	2.661654	0.104882	0.415409	0.196729
5	2.381975	0.093861	0.371759	0.176058
6	1.492067	0.058795	0.232870	0.110282
7	1.652779	0.065127	0.257952	0.122161
8	3.983692	0.156977	0.621742	0.294444
9	0.268165	0.010567	0.041853	0.019821
10	4.796369	0.189000	0.748578	0.354511
11	0.092443	0.003643	0.014428	0.006833
12	47.354853	1.866009	7.390754	3.500111
13	1.411710	0.055628	0.220328	0.104343
14	1.379956	0.054377	0.215372	0.101996
15	0.261390	0.010300	0.040796	0.019320
16	0.310452	0.012233	0.048453	0.022946
17	0.024064	0.000948	0.003756	0.001779
18	1.069063	0.042126	0.166850	0.079017
19	0.062878	0.002478	0.009813	0.004647
20	0.066226	0.002610	0.010336	0.004895
21	0.071577	0.002820	0.011171	0.005290
22	0.046387	0.001828	0.007240	0.003429
23	0.134489	0.005300	0.020990	0.009940
24	0.097621	0.003847	0.015236	0.007215
25	0.276388	0.010891	0.043136	0.020429
26	2.050586	0.080803	0.320039	0.151564
27	0.958859	0.037784	0.149651	0.070872
28	0.217061	0.008553	0.033877	0.016044
29	0.232466	0.009160	0.036281	0.017182
30	0.137975	0.005437	0.021534	0.010198
31	0.072246	0.002847	0.011276	0.005340
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.940480
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CARBON	BALANCE	9.599902 LB AT/MOLN2.	100.03 PERCENT
HYDROGEN	BALANCE	23.268123 LB AT/MOLN2.	96.99 PERCENT
OXYGEN	BALANCE	0.493715 LB AT/MOLN2.	92.87 PERCENT

PERCENT O2 REACT	94.9801	PERCENT C4 REACT	22.2217
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## VII - 53

RUN NO = 18 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.793607	0.031513	0.124892	0.056129
2	0.340094	0.013504	0.053522	0.024054
3	25.183806	1.000000	3.963248	1.781155
4	2.825750	0.112205	0.444696	0.199855
5	2.621752	0.104105	0.412593	0.185427
6	1.701071	0.067546	0.267702	0.120310
7	1.503472	0.059700	0.236606	0.106335
8	4.126814	0.163868	0.649449	0.291874
9	0.300955	0.011950	0.047362	0.021285
10	5.066673	0.201188	0.797357	0.358347
11	0.092694	0.003681	0.014587	0.006556
12	46.280365	1.837703	7.283274	3.273235
13	1.419233	0.056355	0.223349	0.100377
14	1.360622	0.054028	0.214125	0.096232
15	0.285989	0.011356	0.045007	0.020227
16	0.283520	0.011258	0.044618	0.020052
17	0.036572	0.001452	0.005755	0.002587
18	1.045926	0.041532	0.164600	0.073974
19	0.108584	0.004312	0.017088	0.007680
20	0.138558	0.005502	0.021805	0.009800
21	0.091817	0.003646	0.014450	0.006494
22	0.049244	0.001955	0.007750	0.003483
23	0.138063	0.005482	0.021727	0.009765
24	0.099891	0.003966	0.015720	0.007065
25	0.304468	0.012090	0.047915	0.021534
26	2.048157	0.081328	0.322324	0.144858
27	1.022689	0.040609	0.160944	0.072331
28	0.256031	0.010166	0.040292	0.018108
29	0.241567	0.009592	0.038016	0.017085
30	0.135935	0.005398	0.021392	0.009614
31	0.096091	0.003816	0.015122	0.006796
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999994	3.970806
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CARBON	BALANCE	9.617145	LB AT/MOLN2.	100.21	PERCENT
HYDROGEN	BALANCE	23.305055	LB AT/MOLN2.	97.14	PERCENT
OXYGEN	BALANCE	0.500709	LB AT/MOLN2.	94.18	PERCENT

PERCENT O2 REACT	94.9197	PERCENT C4 REACT	23.4015
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RUN NO = 18 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.848626	0.033830	0.133993	0.058818
2	0.334904	0.013351	0.052879	0.023212
3	25.085356	1.000000	3.960832	1.738649
4	2.809107	0.111982	0.443542	0.194697
5	2.598323	0.103579	0.410260	0.180088
6	1.914608	0.076324	0.302306	0.132700
7	1.320038	0.052622	0.208426	0.091491
8	4.498189	0.179315	0.710238	0.311766
9	0.321480	0.012815	0.050760	0.022282
10	5.218077	0.208013	0.823904	0.361661
11	0.102554	0.004088	0.016193	0.007108
12	45.755126	1.823978	7.224469	3.171257
13	1.355660	0.054042	0.214051	0.093960
14	1.367687	0.054521	0.215950	0.094793
15	0.297019	0.011840	0.046898	0.020586
16	0.297765	0.011870	0.047015	0.020638
17	0.042766	0.001705	0.006753	0.002964
18	1.067303	0.042547	0.168521	0.073974
19	0.110804	0.004417	0.017495	0.007680
20	0.128081	0.005106	0.020223	0.008877
21	0.109775	0.004376	0.017333	0.007608
22	0.047128	0.001879	0.007441	0.003266
23	0.118385	0.004719	0.018692	0.008205
24	0.101582	0.004049	0.016039	0.007041
25	0.276851	0.011036	0.043713	0.019188
26	2.101288	0.083766	0.331781	0.145639
27	1.048913	0.041814	0.165617	0.072699
28	0.247598	0.009870	0.039094	0.017161
29	0.239937	0.009565	0.037885	0.016630
30	0.136731	0.005451	0.021589	0.009477
31	0.098345	0.003920	0.015528	0.006816
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.986390
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CARBON	BALANCE	9.627255 LB AT/MOLN2.	100.32 PERCENT
HYDROGEN	BALANCE	23.343416 LB AT/MOLN2.	97.30 PERCENT
OXYGEN	BALANCE	0.489480 LB AT/MOLN2.	92.07 PERCENT

PERCENT O2 REACT	94.9776	PERCENT C4 REACT	23.9736
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## VII - 55

RUN NO = 18 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.850612	0.033699	0.133507	0.058366
2	0.338442	0.013408	0.053120	0.023223
3	25.241432	1.000000	3.961736	1.731988
4	2.769118	0.109705	0.434623	0.190008
5	2.548167	0.100952	0.399944	0.174847
6	1.886636	0.074744	0.296114	0.129455
7	1.250088	0.049525	0.196206	0.085777
8	4.263685	0.168916	0.669201	0.292561
9	0.336093	0.013315	0.052751	0.023062
10	5.170538	0.204843	0.811535	0.354786
11	0.101445	0.004019	0.015922	0.006961
12	45.983972	1.821766	7.217355	3.155276
13	1.396333	0.055319	0.219160	0.095812
14	1.359610	0.053864	0.213396	0.093292
15	0.276247	0.010944	0.043358	0.018955
16	0.288652	0.011436	0.045305	0.019806
17	0.043710	0.001732	0.006860	0.002999
18	1.049387	0.041574	0.164705	0.072006
19	0.109274	0.004329	0.017151	0.007498
20	0.141886	0.005621	0.022269	0.009736
21	0.112947	0.004475	0.017727	0.007750
22	0.059967	0.002376	0.009412	0.004115
23	0.127031	0.005033	0.019938	0.008716
24	0.076714	0.003039	0.012041	0.005264
25	0.300255	0.011895	0.047126	0.020603
26	2.102806	0.083308	0.330043	0.144288
27	1.055747	0.041826	0.165703	0.072442
28	0.272591	0.010799	0.042784	0.018704
29	0.247957	0.009823	0.038918	0.017014
30	0.143669	0.005692	0.022549	0.009858
31	0.094994	0.003763	0.014910	0.006518
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999994	3.961740
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CARBON	BALANCE	9.585227 LB AT/MOLN2.	99.88 PERCENT
HYDROGEN	BALANCE	23.260244 LB AT/MOLN2.	96.95 PERCENT
OXYGEN	BALANCE	0.480326 LB AT/MOLN2.	90.35 PERCENT

PERCENT O2 REACT	94.9560	PERCENT C4 REACT	24.0658
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RUN NO = 19

REACTOR ENTRANCE CONDITIONS

AIR = 2.94 LB/HR BUTANE = 9.46 LB/HR

TEMPERATURE = 685.00 DEG F

PRESSURE = 57.50 LB/SQ IN

OXYGEN = 8.0851 NITROGEN = 30.4152 BUTANE = 61.4997 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0220 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2193 LB/CU FT

GAS VELOCITY = 7.37 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.32 SEC

REYNOLDS NUMBER = 6237



## VII - 57

RUN NO = 19 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.672999	0.023461	0.097725	0.051603
2	0.738646	0.025750	0.107258	0.056637
3	28.685625	1.000000	4.165398	2.199507
4	1.453302	0.050663	0.211032	0.111434
5	1.816508	0.063325	0.263772	0.139283
6	1.902742	0.066331	0.276294	0.145895
7	4.884867	0.170290	0.709325	0.374553
8	6.491978	0.226315	0.942691	0.497781
9	0.269438	0.009393	0.039125	0.020660
10	4.363614	0.152118	0.633634	0.334586
11	0.079125	0.002758	0.011490	0.006067
12	44.960645	1.567358	6.528670	3.447415
13	1.017191	0.035460	0.147705	0.077994
14	1.138617	0.039693	0.165337	0.087305
15	0.080120	0.002793	0.011634	0.006143
16	0.223710	0.007799	0.032485	0.017153
17	0.000000	0.000000	0.000000	0.000000
18	0.246517	0.008594	0.035796	0.018902
19	0.091854	0.003202	0.013338	0.007043
20	0.100282	0.003496	0.014562	0.007689
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.050466	0.001759	0.007328	0.003870
25	0.079708	0.002779	0.011574	0.006112
26	0.438393	0.015283	0.063658	0.033614
27	0.159526	0.005561	0.023165	0.012232
28	0.000000	0.000000	0.000000	0.000000
29	0.054128	0.001887	0.007860	0.004150
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999993	3.486066
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CARBON	BALANCE	8.023982 LB AT/MOLN2.	99.21 PERCENT
HYDROGEN	BALANCE	19.124958 LB AT/MOLN2.	94.58 PERCENT
OXYGEN	BALANCE	0.492692 LB AT/MOLN2.	92.67 PERCENT

PERCENT O2 REACT	90.3132	PERCENT C4 REACT	22.4850
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## VII - 58

RUN NO = 19 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.890027	0.031777	0.126579	0.053448
2	0.413986	0.014781	0.058877	0.024861
3	28.008858	1.000000	3.983393	1.681995
4	2.806940	0.100216	0.399200	0.168563
5	3.011498	0.107519	0.428292	0.180847
6	2.123665	0.075821	0.302026	0.127531
7	3.044213	0.108688	0.432945	0.182812
8	7.027707	0.250910	0.999474	0.422030
9	0.356791	0.012738	0.050742	0.021426
10	5.761941	0.205719	0.819458	0.346018
11	0.068879	0.002459	0.009796	0.004136
12	39.981900	1.427473	5.686188	2.401003
13	1.534474	0.054785	0.218231	0.092149
14	1.615777	0.057688	0.229794	0.097031
15	0.242713	0.008666	0.034518	0.014575
16	0.285046	0.010177	0.040539	0.017118
17	0.000000	0.000000	0.000000	0.000000
18	0.465711	0.016627	0.066233	0.027967
19	0.158113	0.005645	0.022487	0.009495
20	0.117668	0.004201	0.016735	0.007066
21	0.093487	0.003338	0.013296	0.005614
22	0.000000	0.000000	0.000000	0.000000
23	0.137992	0.004927	0.019625	0.008287
24	0.097020	0.003464	0.013798	0.005826
25	0.234947	0.008388	0.033414	0.014109
26	0.693621	0.024764	0.098646	0.041654
27	0.439175	0.015680	0.062459	0.026373
28	0.118133	0.004218	0.016801	0.007094
29	0.137097	0.004895	0.019498	0.008233
30	0.045881	0.001638	0.006525	0.002755
31	0.086744	0.003097	0.012337	0.005209
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.570299
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CARBON	BALANCE	8.039779 LB AT/MOLN2.	99.40 PERCENT
HYDROGEN	BALANCE	19.096233 LB AT/MOLN2.	94.44 PERCENT
OXYGEN	BALANCE	0.457894 LB AT/MOLN2.	86.13 PERCENT

PERCENT O2 REACT	94.4397	PERCENT C4 REACT	29.4031
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VII - 59

RUN NO = 19 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.904782	0.032494	0.129023	0.048528
2	0.389147	0.013976	0.055493	0.020872
3	27.844546	1.000000	3.970663	1.493446
4	2.989832	0.107376	0.426353	0.160360
5	3.188486	0.114510	0.454682	0.171015
6	2.230238	0.080096	0.318034	0.119619
7	2.337397	0.083945	0.333315	0.125367
8	7.626321	0.273889	1.087522	0.409039
9	0.402632	0.014460	0.057416	0.021595
10	6.593574	0.236799	0.940251	0.353647
11	0.084952	0.003051	0.012114	0.004556
12	37.657327	1.352413	5.369977	2.019756
13	1.671552	0.060032	0.238365	0.089654
14	1.667576	0.059889	0.237798	0.089441
15	0.386050	0.013864	0.055051	0.020706
16	0.373181	0.013402	0.053216	0.020016
17	0.068067	0.002445	0.009706	0.003651
18	0.591321	0.021237	0.084323	0.031716
19	0.202476	0.007272	0.028873	0.010860
20	0.176413	0.006336	0.025157	0.009462
21	0.123158	0.004423	0.017563	0.006606
22	0.000000	0.000000	0.000000	0.000000
23	0.162843	0.005848	0.023222	0.008734
24	0.158319	0.005686	0.022577	0.008491
25	0.398882	0.014325	0.056881	0.021394
26	0.826117	0.029669	0.117805	0.044309
27	0.568567	0.020419	0.081078	0.030495
28	0.110135	0.003955	0.015705	0.005907
29	0.133856	0.004807	0.019088	0.007179
30	0.047959	0.001722	0.006839	0.002572
31	0.084300	0.003028	0.012021	0.004521
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999995 3.591367

CARBON	BALANCE	7.991506 LB AT/MOLN2.	98.81 PERCENT
HYDROGEN	BALANCE	18.954969 LB AT/MOLN2.	93.74 PERCENT
OXYGEN	BALANCE	0.447515 LB AT/MOLN2.	84.18 PERCENT

PERCENT O2 REACT 94.7425 PERCENT C4 REACT 33.1153





## VII - 60

RUN NO = 19 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.886431	0.031777	0.126456	0.046102
2	0.405511	0.014537	0.057849	0.021090
3	27.895694	1.000000	3.979528	1.450810
4	2.961541	0.106165	0.422486	0.154025
5	3.227231	0.115689	0.460388	0.167843
6	2.323748	0.083301	0.331500	0.120854
7	2.166503	0.077664	0.309068	0.112676
8	7.852348	0.281490	1.120196	0.408388
9	0.445280	0.015962	0.063522	0.023158
10	6.534933	0.234263	0.932257	0.339871
11	0.081632	0.002926	0.011645	0.004246
12	37.177574	1.332735	5.303657	1.933546
13	1.664351	0.059663	0.237432	0.086560
14	1.736699	0.062257	0.247753	0.090323
15	0.383684	0.013754	0.054735	0.019955
16	0.365722	0.013110	0.052173	0.019021
17	0.072195	0.002588	0.010299	0.003755
18	0.709280	0.025426	0.101184	0.036888
19	0.204762	0.007340	0.029211	0.010649
20	0.170116	0.006098	0.024268	0.008847
21	0.145656	0.005221	0.020779	0.007575
22	0.000000	0.000000	0.000000	0.000000
23	0.182307	0.006535	0.026007	0.009481
24	0.169588	0.006079	0.024193	0.008820
25	0.407030	0.014591	0.058066	0.021169
26	0.793273	0.028437	0.113166	0.041257
27	0.572596	0.020526	0.081685	0.029780
28	0.162865	0.005838	0.023234	0.008470
29	0.142942	0.005124	0.020392	0.007434
30	0.066228	0.002374	0.009448	0.003444
31	0.092287	0.003308	0.013165	0.004800
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999993	3.584782
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CARBON	BALANCE	7.961197 LB AT/MOLN2.	98.43 PERCENT
HYDROGEN	BALANCE	18.881673 LB AT/MOLN2.	93.38 PERCENT
OXYGEN	BALANCE	0.441770 LB AT/MOLN2.	83.09 PERCENT

PERCENT O2 REACT	94.5314	PERCENT C4 REACT	34.0884
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VII - 61

RUN NO = 19 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.914045	0.032994	0.130867	0.047149
2	0.379664	0.013705	0.054358	0.019584
3	27.703401	1.000000	3.966394	1.429014
4	3.000215	0.108298	0.429551	0.154759
5	3.212496	0.115960	0.459944	0.165709
6	2.581530	0.093185	0.369607	0.133162
7	2.317101	0.083640	0.331747	0.119522
8	8.063535	0.291067	1.154485	0.415938
9	0.451692	0.016305	0.064670	0.023299
10	6.563311	0.236914	0.939692	0.338553
11	0.080466	0.002905	0.011521	0.004151
12	36.630056	1.322222	5.244454	1.889475
13	1.663389	0.060043	0.238153	0.085802
14	1.672313	0.060365	0.239431	0.086262
15	0.379732	0.013707	0.054368	0.019588
16	0.373409	0.013479	0.053462	0.019261
17	0.056340	0.002034	0.008066	0.002906
18	0.886360	0.031995	0.126903	0.045721
19	0.201522	0.007274	0.028853	0.010395
20	0.162681	0.005872	0.023292	0.008391
21	0.147987	0.005342	0.021188	0.007634
22	0.000000	0.000000	0.000000	0.000000
23	0.202498	0.007309	0.028992	0.010445
24	0.167205	0.006036	0.023939	0.008625
25	0.415337	0.014992	0.059465	0.021424
26	0.728081	0.026281	0.104242	0.037556
27	0.579558	0.020920	0.082977	0.029895
28	0.161741	0.005838	0.023157	0.008343
29	0.143945	0.005196	0.020609	0.007425
30	0.063597	0.002296	0.009105	0.003281
31	0.096802	0.003494	0.013859	0.004993
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999996 3.609665

CARBON	BALANCE	7.984416 LB AT/MOLN2.	98.72 PERCENT
HYDROGEN	BALANCE	18.910376 LB AT/MOLN2.	93.52 PERCENT
OXYGEN	BALANCE	0.460401 LB AT/MOLN2.	86.60 PERCENT

PERCENT O2 REACT 94.8445 PERCENT C4 REACT 34.6084





VII - 62

RUN NO = 20

REACTOR ENTRANCE CONDITIONS

AIR = 2.94 LB/HR BUTANE = 9.46 LB/HR

TEMPERATURE = 702.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.0851 NITROGEN = 30.4152 BUTANE = 61.4997 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0220 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2010 LB/CU FT

GAS VELOCITY = 8.04 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.21 SEC

REYNOLDS NUMBER = 6158



## VII - 63

RUN NO = 20 SAMPLE NO = 2

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.551115	0.019035	0.076086	0.037601
2	0.452833	0.015641	0.062517	0.030896
3	28.952315	1.000000	3.997088	1.975352
4	2.239627	0.077356	0.309198	0.152805
5	2.466292	0.085185	0.340490	0.168270
6	1.479856	0.051114	0.204305	0.100967
7	2.306104	0.079652	0.318375	0.157340
8	4.001786	0.138220	0.552477	0.273033
9	0.356351	0.012308	0.049197	0.024313
10	4.469271	0.154367	0.617017	0.304928
11	0.072256	0.002496	0.009975	0.004930
12	43.884948	1.515766	6.058652	2.994172
13	1.704282	0.058865	0.235289	0.116279
14	1.679881	0.058022	0.231920	0.114615
15	0.194158	0.006706	0.026805	0.013247
16	0.266267	0.009197	0.036760	0.018167
17	0.015071	0.000521	0.002081	0.001028
18	0.691755	0.023893	0.095502	0.047197
19	0.047666	0.001646	0.006581	0.003252
20	0.000000	0.000000	0.000000	0.000000
21	0.069273	0.002393	0.009564	0.004726
22	0.028723	0.000992	0.003965	0.001960
23	0.085563	0.002955	0.011813	0.005838
24	0.173308	0.005986	0.023926	0.011824
25	0.208763	0.007211	0.028821	0.014243
26	1.925280	0.066498	0.265800	0.131358
27	1.009987	0.034884	0.139436	0.068909
28	0.193206	0.006673	0.026674	0.013182
29	0.242963	0.008392	0.033543	0.016577
30	0.121045	0.004181	0.016711	0.008259
31	0.110069	0.003802	0.015196	0.007510
32	0.000000	0.000000	0.000000	0.000000

TOTALS	100.000001	3.453955
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CARBON	BALANCE	7.961125 LB AT/MOLN2.	98.43 PERCENT
HYDROGEN	BALANCE	19.216692 LB AT/MOLN2.	95.04 PERCENT
OXYGEN	BALANCE	0.448319 LB AT/MOLN2.	84.33 PERCENT

PERCENT O2 REACT	94.1161	PERCENT C4 REACT	25.0365
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## VII - 64

RUN NO = 20 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.596117	0.021431	0.084917	0.038198
2	0.373883	0.013442	0.053260	0.023958
3	27.815085	1.000000	3.962262	1.782349
4	2.779169	0.099916	0.395893	0.178085
5	2.803054	0.100775	0.399295	0.179615
6	1.862077	0.066945	0.265253	0.119319
7	2.581101	0.092795	0.367678	0.165393
8	5.128603	0.184382	0.730570	0.328633
9	0.408742	0.014695	0.058225	0.026192
10	5.561238	0.199936	0.792199	0.356356
11	0.068707	0.002470	0.009787	0.004403
12	40.636393	1.460948	5.788659	2.603919
13	1.649025	0.059285	0.234904	0.105667
14	1.646407	0.059191	0.234531	0.105499
15	0.222029	0.007982	0.031628	0.014227
16	0.291168	0.010468	0.041477	0.018658
17	0.029128	0.001047	0.004149	0.001866
18	0.690542	0.024826	0.098368	0.044249
19	0.088534	0.003183	0.012612	0.005673
20	0.000000	0.000000	0.000000	0.000000
21	0.121743	0.004377	0.017342	0.007801
22	0.034681	0.001247	0.004940	0.002222
23	0.085013	0.003056	0.012110	0.005447
24	0.162375	0.005838	0.023130	0.010405
25	0.182190	0.006550	0.025953	0.011674
26	2.334079	0.083914	0.332490	0.149564
27	1.064197	0.038260	0.151595	0.068192
28	0.208212	0.007486	0.029660	0.013342
29	0.291144	0.010467	0.041473	0.018656
30	0.138668	0.004985	0.019753	0.008886
31	0.146703	0.005274	0.020898	0.009401
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999994	3.595171
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CARBON	BALANCE	8.123963 LB AT/MOLN2.	100.44 PERCENT
HYDROGEN	BALANCE	19.484157 LB AT/MOLN2.	96.36 PERCENT
OXYGEN	BALANCE	0.521496 LB AT/MOLN2.	98.09 PERCENT

PERCENT O2 REACT	94.9434	PERCENT C4 REACT	27.7476
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VII - 65

RUN NO = 20 SAMPLE NO = 5

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.652884	0.023807	0.094546	0.043453
2	0.384355	0.014015	0.055660	0.025581
3	27.423620	1.000000	3.971291	1.825189
4	2.797270	0.102002	0.405080	0.186173
5	3.026542	0.110363	0.438282	0.201433
6	1.780557	0.064928	0.257847	0.118506
7	2.293227	0.083622	0.332089	0.152627
8	5.276857	0.192420	0.764156	0.351203
9	0.423308	0.015436	0.061300	0.028173
10	5.751573	0.209731	0.832901	0.382798
11	0.068538	0.002499	0.009925	0.004562
12	40.425622	1.474117	5.854147	2.690542
13	1.584195	0.057768	0.229412	0.105437
14	1.561037	0.056923	0.226058	0.103895
15	0.222459	0.008112	0.032215	0.014806
16	0.282870	0.010315	0.040963	0.018827
17	0.032417	0.001182	0.004694	0.002158
18	0.560983	0.020456	0.081237	0.037336
19	0.069357	0.002529	0.010044	0.004616
20	0.039084	0.001425	0.005660	0.002601
21	0.182926	0.006670	0.026490	0.012175
22	0.045371	0.001654	0.006570	0.003020
23	0.089052	0.003247	0.012896	0.005927
24	0.154632	0.005639	0.022393	0.010292
25	0.245387	0.008948	0.035535	0.016332
26	2.743418	0.100039	0.397282	0.182589
27	1.061475	0.038707	0.153715	0.070647
28	0.203485	0.007420	0.029467	0.013543
29	0.280685	0.010235	0.040647	0.018681
30	0.151161	0.005512	0.021890	0.010061
31	0.138165	0.005038	0.020008	0.009196
32	0.047494	0.001732	0.006878	0.003161

TOTALS 99.999993 3.646492

CARBON	BALANCE	8.226138 LB AT/MOLN2.	101.71 PERCENT
HYDROGEN	BALANCE	19.797272 LB AT/MOLN2.	97.91 PERCENT
OXYGEN	BALANCE	0.524102 LB AT/MOLN2.	98.58 PERCENT

PERCENT O2 REACT 94.7275 PERCENT C4 REACT 27.0963





RUN NO = 21

REACTOR ENTRANCE CONDITIONS

AIR = 2.98 LB/HR BUTANE = 9.56 LB/HR

TEMPERATURE = 687.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.1000 NITROGEN = 30.4713 BUTANE = 61.4287 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0160 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2036 LB/CU FT

GAS VELOCITY = 8.03 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.21 SEC

REYNOLDS NUMBER = 6295



## VII - 67

RUN NO = 21 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.436092	0.014791	0.059311	0.028811
2	0.484617	0.016437	0.065910	0.032016
3	29.483075	1.000000	4.009853	1.947809
4	1.374009	0.046603	0.186872	0.090774
5	2.571906	0.087233	0.349793	0.169914
6	1.679254	0.056957	0.228387	0.110940
7	5.024873	0.170432	0.683409	0.331970
8	4.502378	0.152711	0.612347	0.297451
9	0.461485	0.015653	0.062764	0.030488
10	5.053902	0.171417	0.687357	0.333888
11	0.082065	0.002783	0.011161	0.005422
12	44.299925	1.502554	6.025023	2.926689
13	0.953157	0.032329	0.129634	0.062971
14	1.100061	0.037312	0.149614	0.072676
15	0.114455	0.003882	0.015566	0.007562
16	0.221324	0.007507	0.030101	0.014622
17	0.031611	0.001072	0.004299	0.002088
18	0.397354	0.013477	0.054042	0.026251
19	0.077513	0.002629	0.010542	0.005121
20	0.072181	0.002448	0.009817	0.004769
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.118429	0.004017	0.016107	0.007824
25	0.096724	0.003281	0.013155	0.006390
26	0.626985	0.021266	0.085273	0.041422
27	0.385850	0.013087	0.052478	0.025491
28	0.112683	0.003822	0.015325	0.007444
29	0.141509	0.004800	0.019246	0.009349
30	0.044921	0.001524	0.006109	0.002968
31	0.051669	0.001752	0.007027	0.003414
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.391776
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CARBON	BALANCE	7.745752 LB AT/MOLN2.	96.06 PERCENT
HYDROGEN	BALANCE	18.503091 LB AT/MOLN2.	91.78 PERCENT
OXYGEN	BALANCE	0.501205 LB AT/MOLN2.	94.27 PERCENT

PERCENT O2 REACT	93.8165	PERCENT C4 REACT	25.4667
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VII - 68

RUN NO = 21 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.601646	0.021331	0.084566	0.040127
2	0.383048	0.013581	0.053840	0.025548
3	28.205276	1.000000	3.964446	1.881183
4	2.275751	0.080685	0.319873	0.151784
5	2.731363	0.096839	0.383912	0.182171
6	1.866950	0.066192	0.262413	0.124518
7	3.861298	0.136900	0.542732	0.257534
8	5.393701	0.191230	0.758122	0.359739
9	0.521985	0.018507	0.073369	0.034814
10	5.708518	0.202392	0.802372	0.380736
11	0.076738	0.002721	0.010786	0.005118
12	41.867100	1.484371	5.884709	2.792373
13	1.486919	0.052718	0.208997	0.099172
14	1.474564	0.052280	0.207260	0.098348
15	0.201383	0.007140	0.028306	0.013431
16	0.243741	0.008642	0.034260	0.016257
17	0.045436	0.001611	0.006386	0.003030
18	0.517969	0.018364	0.072804	0.034547
19	0.092439	0.003277	0.012993	0.006165
20	0.106932	0.003791	0.015030	0.007132
21	0.000000	0.000000	0.000000	0.000000
22	0.057512	0.002039	0.008084	0.003836
23	0.095622	0.003390	0.013440	0.006378
24	0.123861	0.004391	0.017410	0.008261
25	0.201899	0.007158	0.028378	0.013466
26	0.697004	0.024712	0.097969	0.046487
27	0.620341	0.021994	0.087193	0.041374
28	0.148417	0.005262	0.020861	0.009899
29	0.169546	0.006011	0.023831	0.011308
30	0.089192	0.003162	0.012537	0.005949
31	0.133852	0.004746	0.018814	0.008927
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999995 3.545436

CARBON	BALANCE	8.122319 LB AT/MOLN2.	100.73 PERCENT
HYDROGEN	BALANCE	19.317293 LB AT/MOLN2.	95.82 PERCENT
OXYGEN	BALANCE	0.500410 LB AT/MOLN2.	94.12 PERCENT

PERCENT O2 REACT 94.8911 PERCENT C4 REACT 26.3687





RUN NO = 21 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.661490	0.023492	0.093170	0.039610
2	0.385162	0.013679	0.054250	0.023064
3	28.157771	1.000000	3.965987	1.686103
4	2.488006	0.088359	0.350433	0.148983
5	3.031794	0.107672	0.427024	0.181545
6	2.043855	0.072586	0.287874	0.122387
7	2.716542	0.096476	0.382622	0.162668
8	5.961660	0.211723	0.839692	0.356987
9	0.594128	0.021100	0.083682	0.035577
10	6.447599	0.228981	0.908136	0.386086
11	0.076255	0.002708	0.010740	0.004566
12	40.064791	1.422868	5.643076	2.399101
13	1.589011	0.056432	0.223810	0.095151
14	1.615787	0.057383	0.227582	0.096754
15	0.255337	0.009068	0.035964	0.015290
16	0.256506	0.009110	0.036128	0.015360
17	0.045839	0.001628	0.006456	0.002745
18	0.608719	0.021618	0.085737	0.036450
19	0.110092	0.003910	0.015506	0.006592
20	0.131641	0.004675	0.018541	0.007883
21	0.000000	0.000000	0.000000	0.000000
22	0.100001	0.003551	0.014085	0.005988
23	0.119814	0.004255	0.016876	0.007174
24	0.139198	0.004944	0.019606	0.008335
25	0.336581	0.011953	0.047407	0.020155
26	0.731818	0.025990	0.103076	0.043822
27	0.711911	0.025283	0.100272	0.042630
28	0.149795	0.005320	0.021098	0.008970
29	0.198972	0.007066	0.028025	0.011915
30	0.095658	0.003397	0.013473	0.005728
31	0.174274	0.006189	0.024546	0.010436
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.551417
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CARBON	BALANCE	8.083280 LB AT/MOLN2.	100.24 PERCENT
HYDROGEN	BALANCE	19.249165 LB AT/MOLN2.	95.48 PERCENT
OXYGEN	BALANCE	0.447537 LB AT/MOLN2.	84.18 PERCENT

PERCENT O2 REACT	94.8542	PERCENT C4 REACT	29.4195
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## VII - 70

RUN NO = 21 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.713405	0.025443	0.100755	0.041147
2	0.372932	0.013300	0.052670	0.021510
3	28.039465	1.000000	3.960043	1.617229
4	2.557443	0.091209	0.361190	0.147505
5	3.039269	0.108393	0.429239	0.175296
6	2.116724	0.075491	0.298947	0.122086
7	2.813928	0.100356	0.397414	0.162299
8	6.376549	0.227413	0.900567	0.367779
9	0.599101	0.021366	0.084612	0.034554
10	6.445897	0.229887	0.910361	0.371779
11	0.076763	0.002738	0.010841	0.004427
12	39.188237	1.397610	5.534596	2.260255
13	1.610742	0.057446	0.227487	0.092903
14	1.640716	0.058515	0.231720	0.094631
15	0.264209	0.009423	0.037314	0.015239
16	0.241315	0.008606	0.034081	0.013918
17	0.046719	0.001666	0.006598	0.002695
18	0.614676	0.021922	0.086811	0.035453
19	0.118657	0.004232	0.016758	0.006844
20	0.126977	0.004529	0.017933	0.007324
21	0.000000	0.000000	0.000000	0.000000
22	0.100940	0.003600	0.014256	0.005822
23	0.126977	0.004529	0.017933	0.007324
24	0.172635	0.006157	0.024381	0.009957
25	0.460947	0.016439	0.065100	0.026586
26	0.715140	0.025505	0.101000	0.041247
27	0.802502	0.028620	0.113338	0.046286
28	0.179307	0.006395	0.025324	0.010342
29	0.190034	0.006777	0.026839	0.010961
30	0.093098	0.003320	0.013148	0.005370
31	0.154701	0.005517	0.021849	0.008923
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	3.566402
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CARBON	BALANCE	8.055881 LB AT/MOLN2.	99.90 PERCENT
HYDROGEN	BALANCE	19.157478 LB AT/MOLN2.	95.03 PERCENT
OXYGEN	BALANCE	0.466260 LB AT/MOLN2.	87.70 PERCENT

PERCENT O2 REACT	94.9966	PERCENT C4 REACT	30.6724
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## VII - 71

RUN NO = 21 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.764509	0.027479	0.108948	0.044565
2	0.378553	0.013606	0.053947	0.022067
3	27.821974	1.000000	3.964847	1.621819
4	2.579192	0.092703	0.367555	0.150348
5	3.091003	0.111099	0.440492	0.180183
6	2.147088	0.077172	0.305977	0.125160
7	2.888912	0.103836	0.411692	0.168403
8	6.318632	0.227109	0.900454	0.368330
9	0.588663	0.021158	0.083889	0.034315
10	6.426629	0.230991	0.915845	0.374626
11	0.081390	0.002925	0.011599	0.004744
12	38.932959	1.399360	5.548249	2.269509
13	1.590832	0.057179	0.226706	0.092734
14	1.641769	0.059010	0.233965	0.095703
15	0.278934	0.010026	0.039750	0.016260
16	0.264625	0.009511	0.037711	0.015426
17	0.063964	0.002299	0.009115	0.003729
18	0.612795	0.022026	0.087328	0.035721
19	0.131147	0.004714	0.018689	0.007645
20	0.113522	0.004080	0.016178	0.006617
21	0.000000	0.000000	0.000000	0.000000
22	0.117106	0.004209	0.016689	0.006826
23	0.128306	0.004612	0.018285	0.007479
24	0.188609	0.006779	0.026878	0.010995
25	0.583688	0.020979	0.083180	0.034025
26	0.758108	0.027249	0.108036	0.044192
27	0.858892	0.030871	0.122399	0.050067
28	0.160698	0.005776	0.022901	0.009368
29	0.211634	0.007607	0.030159	0.012337
30	0.100767	0.003622	0.014360	0.005874
31	0.175106	0.006294	0.024954	0.010207
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	3.594281
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CARBON	BALANCE	8.104965 LB AT/MOLN2.	100.51 PERCENT
HYDROGEN	BALANCE	19.283124 LB AT/MOLN2.	95.65 PERCENT
OXYGEN	BALANCE	0.487018 LB AT/MOLN2.	91.61 PERCENT

PERCENT O2 REACT	94.8814	PERCENT C4 REACT	30.5856
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VII - 72

RUN NO = 22

REACTOR ENTRANCE CONDITIONS

AIR = 2.90 LB/HR BUTANE = 9.37 LB/HR

TEMPERATURE = 723.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.0645 NITROGEN = 30.3378 BUTANE = 61.5977 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0304 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.1976 LB/CU FT

GAS VELOCITY = 8.10 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.20 SEC

REYNOLDS NUMBER = 6004



VII - 73

RUN NO = 22 SAMPLE NO = 1

PROD NO	MGL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.615233	0.021179	0.085982	0.057079
2	0.566692	0.019508	0.079199	0.052576
3	29.049491	1.000000	4.059843	2.695126
4	2.184866	0.075212	0.305348	0.202705
5	1.352660	0.046564	0.189042	0.125496
6	0.928217	0.031953	0.129724	0.086117
7	3.843641	0.132314	0.537172	0.356602
8	3.523702	0.121300	0.492459	0.326919
9	0.282867	0.009737	0.039532	0.026244
10	2.861612	0.098508	0.399928	0.265492
11	0.099571	0.003428	0.013916	0.009238
12	48.203352	1.659353	6.736711	4.472165
13	1.448168	0.049852	0.202390	0.134357
14	1.798249	0.061903	0.251316	0.166836
15	0.198823	0.006844	0.027787	0.018446
16	0.159063	0.005476	0.022230	0.014757
17	0.000000	0.000000	0.000000	0.000000
18	0.898460	0.030929	0.125565	0.083356
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.048926	0.001684	0.006838	0.004539
24	0.075365	0.002594	0.010533	0.006992
25	0.175234	0.006032	0.024490	0.016258
26	0.768636	0.026460	0.107422	0.071312
27	0.590968	0.020343	0.082591	0.054828
28	0.109334	0.003764	0.015280	0.010144
29	0.216875	0.007466	0.030310	0.020121
30	0.000000	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS 99.999996 3.442401

CARBON	BALANCE	8.167597 LB AT/MOLN2.	100.57 PERCENT
HYDROGEN	BALANCE	19.570240 LB AT/MOLN2.	96.39 PERCENT
OXYGEN	BALANCE	0.490446 LB AT/MOLN2.	92.25 PERCENT

PERCENT O2 REACT 92.6613 PERCENT C4 REACT 18.2743





## VII - 74

RUN NO = 22 SAMPLE NO = 2

PROD NO	MCL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.791183	0.028024	0.111173	0.050125
2	0.388219	0.013751	0.054551	0.024596
3	28.232609	1.000000	3.967120	1.788676
4	3.152915	0.111676	0.443033	0.199753
5	2.845694	0.100795	0.399864	0.180289
6	1.644863	0.058261	0.231129	0.104210
7	2.365343	0.083781	0.332367	0.149856
8	4.573346	0.161988	0.642626	0.289744
9	0.566734	0.020074	0.079635	0.035905
10	5.520996	0.195554	0.775786	0.349782
11	0.094767	0.003357	0.013316	0.006004
12	41.539205	1.471320	5.836903	2.631715
13	1.606948	0.056918	0.225801	0.101808
14	1.968378	0.069720	0.276588	0.124707
15	0.255201	0.009039	0.035860	0.016168
16	0.217671	0.007710	0.030586	0.013791
17	0.036417	0.001290	0.005117	0.002307
18	0.923613	0.032714	0.129782	0.058515
19	0.035242	0.001248	0.004952	0.002233
20	0.068355	0.002421	0.009605	0.004331
21	0.022458	0.000795	0.003156	0.001423
22	0.070532	0.002498	0.009911	0.004469
23	0.122833	0.004351	0.017260	0.007782
24	0.103745	0.003675	0.014578	0.006573
25	0.284819	0.010088	0.040022	0.018045
26	1.123107	0.039780	0.157814	0.071154
27	0.834305	0.029551	0.117233	0.052857
28	0.195299	0.006918	0.027443	0.012373
29	0.231590	0.008203	0.032542	0.014672
30	0.087185	0.003088	0.012251	0.005524
31	0.096435	0.003416	0.013551	0.006110
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999994	3.542003
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CARBON	BALANCE	8.098587 LB AT/MOLN2.	99.72 PERCENT
HYDROGEN	BALANCE	19.346599 LB AT/MOLN2.	95.28 PERCENT
OXYGEN	BALANCE	0.467693 LB AT/MOLN2.	87.97 PERCENT

PERCENT O2 REACT	94.8271	PERCENT C4 REACT	27.5352
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## VII - 75

RUN NO = 22 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.836622	0.029534	0.117115	0.048356
2	0.386483	0.013643	0.054102	0.022338
3	28.327347	1.000000	3.965432	1.637283
4	3.245965	0.114588	0.454390	0.187612
5	3.039186	0.107288	0.425444	0.175661
6	1.893487	0.066843	0.265062	0.109441
7	1.871381	0.066063	0.261967	0.108163
8	4.712839	0.166371	0.659731	0.272396
9	0.639203	0.022565	0.089480	0.036945
10	5.749659	0.202972	0.804872	0.332323
11	0.081523	0.002878	0.011412	0.004712
12	40.214203	1.419625	5.629425	2.324327
13	1.602036	0.056554	0.224263	0.092596
14	1.982464	0.069984	0.277517	0.114584
15	0.279041	0.009851	0.039062	0.016128
16	0.244473	0.008630	0.034223	0.014130
17	0.061152	0.002159	0.008560	0.003535
18	0.991765	0.035011	0.138833	0.057323
19	0.062409	0.002203	0.008736	0.003607
20	0.094006	0.003319	0.013159	0.005433
21	0.020696	0.000731	0.002897	0.001196
22	0.066505	0.002348	0.009310	0.003844
23	0.140734	0.004968	0.019701	0.008134
24	0.105857	0.003737	0.014819	0.006118
25	0.347036	0.012251	0.048580	0.020058
26	1.307805	0.046168	0.183074	0.075589
27	0.949219	0.033509	0.132877	0.054864
28	0.233759	0.008252	0.032723	0.013511
29	0.232013	0.008190	0.032479	0.013410
30	0.142005	0.005013	0.019879	0.008208
31	0.139134	0.004912	0.019477	0.008042
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999997	3.530158
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CARBON	BALANCE	7.985260 LB AT/MOLN2.	98.32 PERCENT
HYDROGEN	BALANCE	19.115445 LB AT/MOLN2.	94.15 PERCENT
OXYGEN	BALANCE	0.457810 LB AT/MOLN2.	86.11 PERCENT

PERCENT O2 REACT	94.8675	PERCENT C4 REACT	30.0813
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## VII - 76

RUN NO = 22 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.890784	0.031646	0.125501	0.051705
2	0.384641	0.013665	0.054191	0.022326
3	28.148326	1.000000	3.965767	1.633840
4	3.249326	0.115436	0.457792	0.188604
5	3.047735	0.108274	0.429390	0.176903
6	1.872011	0.066505	0.263744	0.108659
7	1.847637	0.065639	0.260310	0.107244
8	4.823323	0.171354	0.679549	0.279965
9	0.663632	0.023576	0.093498	0.038520
10	5.944326	0.211179	0.837485	0.345032
11	0.078833	0.002801	0.011107	0.004576
12	39.923836	1.418338	5.624798	2.317337
13	1.599309	0.056817	0.225324	0.092830
14	1.960091	0.069634	0.276154	0.113771
15	0.277891	0.009872	0.039152	0.016130
16	0.245263	0.008713	0.034555	0.014236
17	0.054587	0.001939	0.007691	0.003168
18	1.016177	0.036101	0.143167	0.058983
19	0.071415	0.002537	0.010062	0.004145
20	0.088346	0.003139	0.012447	0.005128
21	0.023539	0.000836	0.003316	0.001366
22	0.067271	0.002390	0.009478	0.003905
23	0.135212	0.004804	0.019050	0.007848
24	0.093206	0.003311	0.013132	0.005410
25	0.342412	0.012165	0.048242	0.019875
26	1.394929	0.049556	0.196529	0.080967
27	0.958872	0.034065	0.135094	0.055657
28	0.248267	0.008820	0.034978	0.014410
29	0.240103	0.008530	0.033828	0.013937
30	0.153170	0.005442	0.021580	0.008891
31	0.155535	0.005526	0.021913	0.009028
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999995	3.552609
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CARBON	BALANCE	8.028337 LB AT/MOLN2.	98.85 PERCENT
HYDROGEN	BALANCE	19.214663 LB AT/MOLN2.	94.64 PERCENT
OXYGEN	BALANCE	0.464087 LB AT/MOLN2.	87.29 PERCENT

PERCENT O2 REACT	94.8594	PERCENT C4 REACT	30.1447
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## VII - 77

RUN NO = 22 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.920025	0.032645	0.129252	0.052974
2	0.373465	0.013252	0.052467	0.021504
3	28.182374	1.000000	3.959282	1.622697
4	3.222139	0.114332	0.452671	0.185526
5	3.042866	0.107971	0.427486	0.175203
6	1.877616	0.066624	0.263782	0.108110
7	1.691072	0.060005	0.237575	0.097369
8	4.809472	0.170655	0.675673	0.276922
9	0.658836	0.023378	0.092558	0.037935
10	6.072940	0.215487	0.853175	0.349670
11	0.081017	0.002875	0.011382	0.004665
12	39.853679	1.414135	5.598959	2.294712
13	1.610631	0.057150	0.226274	0.092738
14	2.033769	0.072165	0.285720	0.117101
15	0.260384	0.009239	0.036581	0.014993
16	0.248185	0.008806	0.034867	0.014290
17	0.048730	0.001729	0.006846	0.002806
18	1.052507	0.037346	0.147865	0.060602
19	0.076631	0.002719	0.010766	0.004412
20	0.092842	0.003294	0.013043	0.005346
21	0.030167	0.001070	0.004238	0.001737
22	0.070114	0.002488	0.009850	0.004037
23	0.147000	0.005216	0.020652	0.008464
24	0.116112	0.004120	0.016312	0.006686
25	0.342108	0.012139	0.048062	0.019698
26	1.433349	0.050860	0.201368	0.082530
27	0.923261	0.032760	0.129707	0.053160
28	0.232329	0.008244	0.032639	0.013377
29	0.219368	0.007784	0.030819	0.012631
30	0.135224	0.004798	0.018997	0.007786
31	0.141795	0.005031	0.019920	0.008164
32	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999996	3.548317		

CARBON	BALANCE	8.023104 LB AT/MOLN2.	98.79 PERCENT
HYDROGEN	BALANCE	19.209916 LB AT/MOLN2.	94.61 PERCENT
OXYGEN	BALANCE	0.450483 LB AT/MOLN2.	84.73 PERCENT

PERCENT O2 REACT	95.0148	PERCENT C4 REACT	30.3517
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VII - 78

RUN NO = 26

REACTOR ENTRANCE CONDITIONS

AIR = 2.95 LB/HR BUTANE = 9.43 LB/HR

TEMPERATURE = 699.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.1178 NITROGEN = 30.5382 BUTANE = 61.3440 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0088 MOLS/MN2

DENSITY OF GAS MIXTURE = 0.2014 LB/CU FT

GAS VELOCITY = 8.02 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.22 SEC

REYNOLDS NUMBER = 6156



## VII - 79

RUN NO = 26 SAMPLE NO = 1

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	4.289371	0.140012	1.112885	0.602378
3	30.635648	1.000000	7.948471	4.302320
4	0.735248	0.024000	0.190761	0.103255
5	0.533078	0.017401	0.138308	0.074863
6	0.374485	0.012224	0.097161	0.052591
7	2.030746	0.066287	0.526881	0.285188
8	1.048984	0.034241	0.272161	0.147314
9	0.036037	0.001176	0.009350	0.005061
10	0.820980	0.026798	0.213005	0.115294
11	0.116996	0.003819	0.030355	0.016430
12	54.418953	1.776328	14.119091	7.642331
13	1.351185	0.044105	0.350567	0.189754
14	1.401453	0.045746	0.363609	0.196813
15	0.000000	0.000000	0.000000	0.000000
16	0.162956	0.005319	0.042279	0.022885
17	0.000000	0.000000	0.000000	0.000000
18	0.358374	0.011698	0.092981	0.050328
19	0.000000	0.000000	0.000000	0.000000
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.077828	0.002540	0.020193	0.010930
25	0.081806	0.002670	0.021225	0.011488
26	0.761306	0.024850	0.197522	0.106914
27	0.433821	0.014161	0.112556	0.060924
28	0.085282	0.002784	0.022127	0.011977
29	0.178714	0.005834	0.046368	0.025098
30	0.066753	0.002179	0.017319	0.009374
31	0.000000	0.000000	0.000000	0.000000
32	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999996	3.264171
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CARBON	BALANCE	7.878183 LB AT/MOLN2.	98.05 PERCENT
HYDROGEN	BALANCE	19.285406 LB AT/MOLN2.	96.01 PERCENT
OXYGEN	BALANCE	0.508634 LB AT/MOLN2.	95.67 PERCENT

PERCENT O2 REACT	47.3287	PERCENT C4 REACT	11.5710
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## VII - 80

RUN NO = 26 SAMPLE NO = 2

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.525825	0.018266	0.072941	0.036774
2	0.443227	0.015397	0.061483	0.030998
3	28.786677	1.000000	3.993198	2.013240
4	2.281757	0.079264	0.316518	0.159578
5	2.463405	0.085574	0.341716	0.172282
6	1.549722	0.053835	0.214973	0.108382
7	2.040935	0.070899	0.283112	0.142736
8	4.445766	0.154438	0.616703	0.310921
9	0.322608	0.011207	0.044751	0.022562
10	4.638199	0.161123	0.643396	0.324380
11	0.074990	0.002605	0.010402	0.005245
12	43.526864	1.512049	6.037911	3.044118
13	1.637801	0.056894	0.227191	0.114542
14	1.631319	0.056669	0.226291	0.114089
15	0.213365	0.007412	0.029597	0.014922
16	0.280329	0.009738	0.038886	0.019605
17	0.000000	0.000000	0.000000	0.000000
18	0.688995	0.023935	0.095575	0.048186
19	0.046485	0.001615	0.006448	0.003251
20	0.053805	0.001869	0.007464	0.003763
21	0.070405	0.002446	0.009766	0.004924
22	0.030933	0.001075	0.004291	0.002163
23	0.085031	0.002954	0.011795	0.005947
24	0.176520	0.006132	0.024486	0.012345
25	0.199149	0.006918	0.027625	0.013928
26	1.992408	0.069213	0.276381	0.139342
27	1.039805	0.036121	0.144239	0.072720
28	0.209289	0.007270	0.029032	0.014637
29	0.260006	0.009032	0.036067	0.018184
30	0.121316	0.004214	0.016829	0.008484
31	0.112502	0.003908	0.015606	0.007868
32	0.050569	0.001757	0.007015	0.003537

TOTALS	99.999992	3.473829
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CARBON	BALANCE	8.002542 LB AT/MOLN2.	99.60 PERCENT
HYDROGEN	BALANCE	19.318545 LB AT/MOLN2.	96.17 PERCENT
OXYGEN	BALANCE	0.442329 LB AT/MOLN2.	83.20 PERCENT

PERCENT O2 REACT	94.2078	PERCENT C4 REACT	24.7273
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## VII - 81

RUN NO = 26 SAMPLE NO = 3

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.586146	0.021014	0.083345	0.038354
2	0.381972	0.013694	0.054313	0.024994
3	27.893528	1.000000	3.966226	1.825196
4	2.690587	0.096459	0.382579	0.176057
5	2.834547	0.101620	0.403049	0.185477
6	1.839710	0.065955	0.261591	0.120380
7	2.559301	0.091753	0.363911	0.167466
8	5.126659	0.183794	0.728968	0.335460
9	0.394054	0.014127	0.056031	0.025785
10	5.483510	0.196587	0.779709	0.358810
11	0.076709	0.002750	0.010907	0.005019
12	40.748938	1.460874	5.794157	2.666382
13	1.642508	0.058885	0.233551	0.107477
14	1.654777	0.059325	0.235295	0.108279
15	0.228496	0.008192	0.032490	0.014952
16	0.299613	0.010741	0.042602	0.019605
17	0.029765	0.001067	0.004232	0.001948
18	0.640422	0.022960	0.091063	0.041906
19	0.092308	0.003309	0.013125	0.006040
20	0.078627	0.002819	0.011180	0.005145
21	0.121009	0.004338	0.017206	0.007918
22	0.037631	0.001349	0.005351	0.002462
23	0.087528	0.003138	0.012446	0.005727
24	0.158242	0.005673	0.022501	0.010354
25	0.207153	0.007427	0.029455	0.013555
26	2.186240	0.078378	0.310865	0.143055
27	1.059343	0.037978	0.150630	0.069317
28	0.229193	0.008217	0.032589	0.014997
29	0.297915	0.010680	0.042361	0.019494
30	0.144896	0.005195	0.020603	0.009481
31	0.139541	0.005003	0.019842	0.009131
32	0.049138	0.001762	0.006987	0.003215
TOTALS	99.999991	3.585061		

CARBON	BALANCE	8.121910	LB AT/MOLN2.	101.08	PERCENT
HYDROGEN	BALANCE	19.481682	LB AT/MOLN2.	96.98	PERCENT
OXYGEN	BALANCE	0.515513	LB AT/MOLN2.	96.97	PERCENT

PERCENT O2 REACT	94.8485	PERCENT C4 REACT	27.2748
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## VII - 82

RUN NO = 26 SAMPLE NO = 4

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.661909	0.023654	0.093884	0.041887
2	0.388210	0.013873	0.055063	0.024567
3	27.982893	1.000000	3.969047	1.770826
4	2.734525	0.097721	0.387860	0.173047
5	2.971482	0.106189	0.421470	0.188043
6	1.819123	0.065008	0.258021	0.115119
7	2.589386	0.092535	0.367274	0.163863
8	5.275486	0.188525	0.748266	0.333846
9	0.408112	0.014584	0.057886	0.025826
10	5.217646	0.186458	0.740062	0.330185
11	0.079172	0.002829	0.011230	0.005010
12	40.408761	1.444052	5.731511	2.557165
13	1.574987	0.056284	0.223394	0.099669
14	1.648104	0.058897	0.233764	0.104296
15	0.220515	0.007880	0.031277	0.013955
16	0.288704	0.010317	0.040949	0.018270
17	0.032581	0.001164	0.004621	0.002062
18	0.559461	0.019993	0.079353	0.035404
19	0.075899	0.002712	0.010765	0.004803
20	0.078236	0.002796	0.011097	0.004951
21	0.147006	0.005253	0.020851	0.009303
22	0.044248	0.001581	0.006276	0.002800
23	0.120512	0.004307	0.017093	0.007626
24	0.138322	0.004943	0.019619	0.008753
25	0.239611	0.008563	0.033986	0.015163
26	2.371371	0.084744	0.336351	0.150066
27	1.089578	0.038937	0.154544	0.068951
28	0.226489	0.008094	0.032125	0.014333
29	0.288389	0.010306	0.040905	0.018250
30	0.142385	0.005088	0.020196	0.009010
31	0.126167	0.004509	0.017895	0.007984
32	0.050742	0.001813	0.007197	0.003211
TOTALS	99.999999	3.573612		

CARBON	BALANCE	8.025016 LB AT/MOLN2.	99.88 PERCENT
HYDROGEN	BALANCE	19.281868 LB AT/MOLN2.	95.99 PERCENT
OXYGEN	BALANCE	0.522826 LB AT/MOLN2.	98.34 PERCENT

PERCENT O2 REACT	94.7811	PERCENT C4 REACT	28.1123
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RUN NO = 26 SAMPLE NO = 5

PROD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.662855	0.023888	0.094941	0.041689
2	0.394399	0.014213	0.056490	0.024805
3	27.748312	1.000000	3.974415	1.745164
4	2.790303	0.100558	0.399658	0.175490
5	3.044590	0.109722	0.436079	0.191482
6	1.825135	0.065775	0.261416	0.114788
7	2.379529	0.085754	0.340822	0.149655
8	5.377516	0.193796	0.770226	0.338206
9	0.444567	0.016021	0.063676	0.027960
10	5.673388	0.204459	0.812604	0.356814
11	0.073000	0.002631	0.010456	0.004591
12	39.839601	1.435749	5.706261	2.505617
13	1.561959	0.056290	0.223721	0.098236
14	1.577737	0.056859	0.225981	0.099228
15	0.240099	0.008653	0.034390	0.015100
16	0.299544	0.010795	0.042904	0.018839
17	0.030880	0.001113	0.004423	0.001942
18	0.556668	0.020061	0.079732	0.035010
19	0.072449	0.002611	0.010377	0.004557
20	0.042609	0.001536	0.006103	0.002680
21	0.183045	0.006597	0.026218	0.011512
22	0.045963	0.001656	0.006583	0.002891
23	0.090413	0.003258	0.012950	0.005686
24	0.154193	0.005557	0.022085	0.009698
25	0.250928	0.009043	0.035941	0.015782
26	2.667003	0.096114	0.381997	0.167735
27	1.092928	0.039387	0.156541	0.068737
28	0.226824	0.008174	0.032488	0.014266
29	0.299893	0.010808	0.042954	0.018861
30	0.155259	0.005595	0.022238	0.009765
31	0.142847	0.005148	0.020460	0.008984
32	0.055572	0.002003	0.007960	0.003495

TOTALS	99.999994	3.603823
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CARBON	BALANCE	8.066565 LB AT/MOLN2.	100.39 PERCENT
HYDROGEN	BALANCE	19.396315 LB AT/MOLN2.	96.56 PERCENT
OXYGEN	BALANCE	0.526624 LB AT/MOLN2.	99.06 PERCENT

PERCENT O2 REACT	94.6530	PERCENT C4 REACT	28.5256
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The experimental product distribution for each sample were determined by the method outlined in Appendix VI and are given here. Each run is separate and initial conditions are given along with the analysis. The run numbers correspond to the ones given in Table 1. Component numbers correspond to the list below.

Table VII-1

Components Separated

<u>Component Number</u>	<u>Component Name</u>
1	Hydrogen
2	Oxygen
3	Nitrogen
4	Carbon Monoxide
5	Methane
6	Ethane
7	Carbon Dioxide
8	Ethylene
9	Propane
10	Propylene
11	i-Butane
12	n-Butane
13	1-Butene
14	2-Butene
15	Formaldehyde
16	Ethylene Oxide
17	2-Methyl Butane
18	Acetaldehyde
19	n-Pentane
20	Propylene Oxide
21	3-Methyl Pentane



<u>Component Number</u>	<u>Component Name</u>
22	n-Hexane
23	Propionaldehyde
24	Acetone
25	Methanol
26	Water
27	Ethanol
28	Butyraldehyde
29	Methyl Ethyl Ketone
30	n-Propanol
31	Diethyl Ketone
32	n-Butanol





## APPENDIX VIII

### CARBON AND HYDROGEN BALANCES BASED ON THE N-BUTANE REACTED



Carbon and hydrogen balances may also be calculated on the basis of the n-butane reacted for each product sample. The procedure used to calculate these balances is outlined below.

Calculate the lb. atoms of carbon and hydrogen in each product sample, not including n-butane and i-butane.

Determine the lb-moles of butane reacted for each sample.

$$\% \text{ Carbon Balance} = \frac{100 \times \text{lb. atoms of carbon in product}}{4 \times \text{lb. moles of butane reacted}}$$

$$\% \text{ Hydrogen Balance} = \frac{100 \times \text{lb. atoms of hydrogen in product}}{10 \times \text{lb. moles of butane reacted}}$$

The Carbon and Hydrogen balances are given in Tables VIII-1 and VIII-2 respectively.

The carbon balances based on the butane reacted ranged between 83 and 124 per cent for all samples with the majority of the balances being between 95 and 102 per cent. The carbon balance for samples 2 to 5 for all runs indicate that at relatively high butane conversions, the analyses seem to be reliable. However, the large fluctuations in the carbon balance for sample 1 for many of the runs indicate that a more accurate analysis was required at low butane conversions. A more sensitive chromatography unit and a more accurate calibration would be needed if good analyses are to be





obtained in these regions.

All hydrogen balances based on the butane converted were low, between 80 and 90 per cent. This fact, coupled with the low oxygen balances discussed earlier and the poor resolution of the water peak observed on the chromatograms, suggested a low water analysis in the product samples.

The low hydrogen balances also indicated that the analysis technique for hydrogen was poor and that more hydrogen was present in the samples than indicated by the gas chromatograph. Once again, a more sensitive chromatograph with a carrier gas other than helium or a detector other than a thermal detector would provide accurate analysis for the hydrogen.



Table VIII-1Carbon Balance Based on the Butane Reacted

Sample No.	1	2	3	4	5
<u>Run No.</u>	<u>% Carbon Balance</u>				
10	97.0	92.2	97.6	97.7	98.5
11	104.5	96.5	96.5	94.4	101.5
12	103.5	123.8*	97.7	94.7	96.9
13	88.1	103.2	93.8	88.9	99.0
14	87.5	101.4	99.1	94.2	104.0
15	85.6	101.4	101.9	92.4	101.0
16	98.0	97.6	100.3	97.8	101.7
17	103.1	103.2	104.2	97.9	99.7
18	100.0	100.1	100.9	101.4	99.5
19	96.5	98.0	96.4	95.4	96.3
20		93.7	101.6		102.3
21	84.4	102.8	100.8	99.7	101.7
22	103.1	99.0	94.4	96.2	96.0
26	83.8	98.3	104.0	99.5	101.4
Aver. % Error	7.2	2.8	2.7	4.0	2.0

\* This reading excluded





Table VIII-2Hydrogen Balance Based on the Butane Reacted

Sample No.	1	2	3	4	5
<u>Run No.</u>	<u>% Hydrogen Balance</u>				
10	82.4	78.6	83.7	84.3	85.2
11	91.8	83.9	84.9	82.8	89.4
12	85.7	105.5	85.5	82.9	84.7
13	78.7	94.1	80.5	77.1	85.5
14	80.3	87.9	84.4	80.8	89.8
15	79.2	87.4	89.9	80.9	89.2
16	85.2	81.8	86.1	84.1	87.9
17	81.3	81.2	94.2	90.6	84.1
18	82.5	86.3	87.7	88.7	87.2
19	85.8	81.0	81.0	80.5	81.2
20		80.1	86.8		92.2
21	77.6	84.1	84.6	83.7	85.7
22	80.0	82.8	80.4	82.1	82.2
26	74.9	84.4	88.9	85.7	87.9



## APPENDIX IX

### RESIDENCE TIME CALCULATIONS





The residence time for each experimental run was calculated as a function of the inlet gas velocity and the change in the reaction temperature, the number of moles, and the molecular weight as the reaction proceeded.

The inlet gas velocity was calculated from the relationship

$$u_o = \frac{\omega}{3600 A \rho_o}$$

where

$u_o$  = entrance velocity, ft/sec

$\omega$  = mass flow rate of the reactants, lb/hr

$A$  = cross-sectional area of the reactor, ft<sup>2</sup>

$\rho_o$  = density of the reaction mixture at the entrance, lb/ft<sup>3</sup>

Therefore,

$$\frac{u}{u_o} = \frac{\omega}{3600 A \rho} \times \frac{3600 A \rho_o}{\omega}$$

$$\frac{u}{u_o} = \frac{\rho_o}{\rho}$$

where

$u$  = velocity at any point in the reactor, ft/sec

$\rho$  = density of the reaction mixture at the point at which the velocity is  $u$ , lb/ft<sup>3</sup>

Using the Ideal Gas Law,

$$\frac{u}{u_o} = \frac{M_o P_o}{n_o RT_o} \times \frac{nRT}{MP}$$



where

M = molecular weight

P = reaction pressure psia

n = number of moles

R = gas constant

T = reaction temperature

subscript o refers to inlet conditions

Therefore

$$u = u_o \left( \frac{M_o}{M} \times \frac{n}{n_o} \times \frac{T}{T_o} \right)$$

The residence time was calculated using the relationship

$$\tau = \int_0^x \frac{dx}{u}$$

where

x = reactor distance, ft.

$\tau$  = residence time in seconds

The velocity at each sample point and the reactor entrance are given in Table IX-1. The residence times for the reacting stream at each sample point are presented in Table IX-2.

The velocity of the reacting gas stream increased up to 60 per cent in the reaction zone and, as a result, the residence time in the reactor was less than the value calculated from the entrance conditions. All reaction parameters, namely, the increase in temperature and the number of moles and





the decrease in the molecular weight of the components decreased the residence time.

All figures in the discussion of results with residence time as a coordinate axis, Figures 9 to 15 and Figures 17 to 23, were plotted with residence times based on inlet conditions. Correct plots should include the residence time calculated from the inlet conditions, the change in the reaction temperature, the number of moles, and the molecular weight.



Table IX-1Reacting Stream Velocity at Each Sample Point

Sample Point	Ent.	1	2	3	4	5
<u>Run No.</u>		<u>Velocity, ft/sec</u>				
10	6.42	10.20	10.15	9.98	9.69	9.31
11	7.09	8.26	9.85	9.77	9.63	9.48
12	8.38	8.37	11.85	11.78	11.60	11.38
13	7.57	8.31	10.68	10.36	10.17	10.07
14	7.52	7.44	10.72	10.52	10.42	10.22
15	7.74	9.83	9.92	9.76	9.58	9.40
16	8.02	9.95	12.24	12.17	11.78	11.54
17	7.95	7.83	8.06	11.76	11.68	11.24
18	8.01	11.52	11.80	11.58	11.47	11.06
19	7.37	10.15	12.28	12.22	12.02	11.77
20	8.04		12.40	12.71		12.08
21	8.03	9.93	13.16	12.78	12.64	12.37
22	8.10	12.17	12.50	12.18	11.83	11.47
26	8.02	9.13	12.45	12.53	12.23	12.02





Table IX-2Residence Time for the Reacting Gas Stream

Sample Point	1	2	3	4	5
Run No.	<u>Residence Time, Sec.</u>				
10	.323	.498	.675	.856	1.043
11	.333	.531	.712	.895	1.081
12	.303	.484	.635	.788	.943
13	.321	.511	.680	.853	1.029
14	.339	.542	.710	.880	1.051
15	.294	.474	.655	.839	1.026
16	.286	.448	.595	.743	.896
17	.321	.545	.731	.883	1.038
18	.270	.423	.575	.730	.888
19	.297	.457	.602	.749	.899
20		.443	.585		.871
21	.286	.443	.580	.720	.862
22	.262	.406	.550	.699	.852
26	.297	.466	.619	.763	.910







**B29849**